LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

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\82X011122W.M
Title : SW846 8260

Signal : TIC: VX026637.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	52	rVB	9530	10282	1.55%	0.200%
2	1.758	104	110	120	rBV	164206	229221	34.47%	4.454%
3	2.349	199	207	222	rVB	20386	43528	6.55%	0.846%
4	2.569	235	243	258	rVB	3100	10890	1.64%	0.212%
5	2.788	269	279	285	rBV	56222	129253	19.44%	2.511%
6	3.105	323	331	345	rVB	81921	184932	27.81%	3.593%
7	4.221	499	514	522	rBV4	9504	29601	4.45%	0.575%
8	4.306	522	528	540	rVB2	3977	11516	1.73%	0.224%
9	5.117	651	661	676	rBV7	3865	17544	2.64%	0.341%
10	5.391	694	706	719	rBV	76920	221527	33.32%	4.304%
11	5.556	723	733	741	rBV	131945	379655	57.10%	7.377%
12	5.842	772	780	789	rBV6	4050	13177	1.98%	0.256%
13	5.958	789	799	809	rVV	86510	228607	34.38%	4.442%
14	6.044	809	813	824	rVV3	8584	22081	3.32%	0.429%
15	6.165	824	833	840	rVV5	13881	44780	6.73%	0.870%
16	6.257	840	848	858	rVV4	27003	83803	12.60%	1.628%
17	6.367	858	866	874	rVB4	4127	11610	1.75%	0.226%
18	6.763	922	931	943	rBV	206171	493542	74.23%	9.590%
19	7.366	1022	1030	1039	rBV6	4936	12772	1.92%	0.248%
20	7.988	1122	1132	1139	rVB2	11306	25977	3.91%	0.505%
21	8.110	1145	1152	1162	rBV2	22303	50408	7.58%	0.979%
22	8.507	1213	1217	1224	rVB3	5149	9767	1.47%	0.190%
23	8.610	1227	1234	1235	rBV3	5613	8920	1.34%	0.173%
24	8.653	1235	1241	1250	rVB	418878	664918	100.00%	12.920%
25	8.842	1266	1272	1278	rVB2	5358	10005	1.50%	0.194%
26	9.104	1307	1315	1320	rBV3	4760	7870	1.18%	0.153%
27	9.165	1320	1325	1336	rVV	7484	11651	1.75%	0.226%
28	9.275	1336	1343	1348	rVV	13980	19320	2.91%	0.375%
29	10.055	1465	1471	1477	rVB	426736	556288	83.66%	10.809%
30	10.963	1613	1620	1627	rBV	66649	84863	12.76%	1.649%
31	11.079	1634	1639	1646	rBV	300424	399138	60.03%	7.755%
32	11.616	1722	1727	1732	rBV	10410	13145	1.98%	0.255%
33	11.866	1764	1768	1770	rBV	7792	9675	1.46%	0.188%
34	11.890	1770	1772	1778	rVB	10988	12118	1.82%	0.235%
35	12.024	1788	1794	1801	rBV	363468	457741	68.84%	8.894%
36	12.244	1824	1830	1837	rBV2	54117	72064	10.84%	1.400%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

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\82X011122W.M
Title : SW846 8260

37	12.317	1837	1842	1843	rVV2	6579	8872	1.33%	0.172%
38	12.335	1843	1845	1850	rVB	8079	8654	1.30%	0.168%
39	12.408	1852	1857	1862	rBV2	11208	13565	2.04%	0.264%
40	12.530	1873	1877	1882	rVB	7039	8348	1.26%	0.162%
41	12.616	1886	1891	1894	rVV	21714	25971	3.91%	0.505%
42	12.701	1900	1905	1912	rVB	92060	112367	16.90%	2.183%
43	12.920	1933	1941	1945	rBV2	5902	8142	1.22%	0.158%
44	13.170	1979	1982	1986	rVV	17885	19819	2.98%	0.385%
45	13.292	1997	2002	2008	rVB2	90810	116572	17.53%	2.265%
46	13.426	2020	2024	2028	rVB	8421	10613	1.60%	0.206%
47	13.542	2040	2043	2047	rVV	13217	18083	2.72%	0.351%
48	13.585	2047	2050	2056	rVV4	9555	18012	2.71%	0.350%
49	13.640	2056	2059	2061	rVV2	7978	11767	1.77%	0.229%
50	13.664	2061	2063	2070	rVB2	15049	19657	2.96%	0.382%
51	13.774	2075	2081	2090	rBV	61582	82100	12.35%	1.595%
52	13.871	2092	2097	2102	rVB	8537	10673	1.61%	0.207%
53	14.079	2127	2131	2135	rBB	5933	6867	1.03%	0.133%
54	14.213	2149	2153	2160	rBV	5806	8379	1.26%	0.163%
55	14.640	2219	2223	2229	rVB	19209	22770	3.42%	0.442%
56	14.780	2242	2246	2254	rBV	17135	23125	3.48%	0.449%

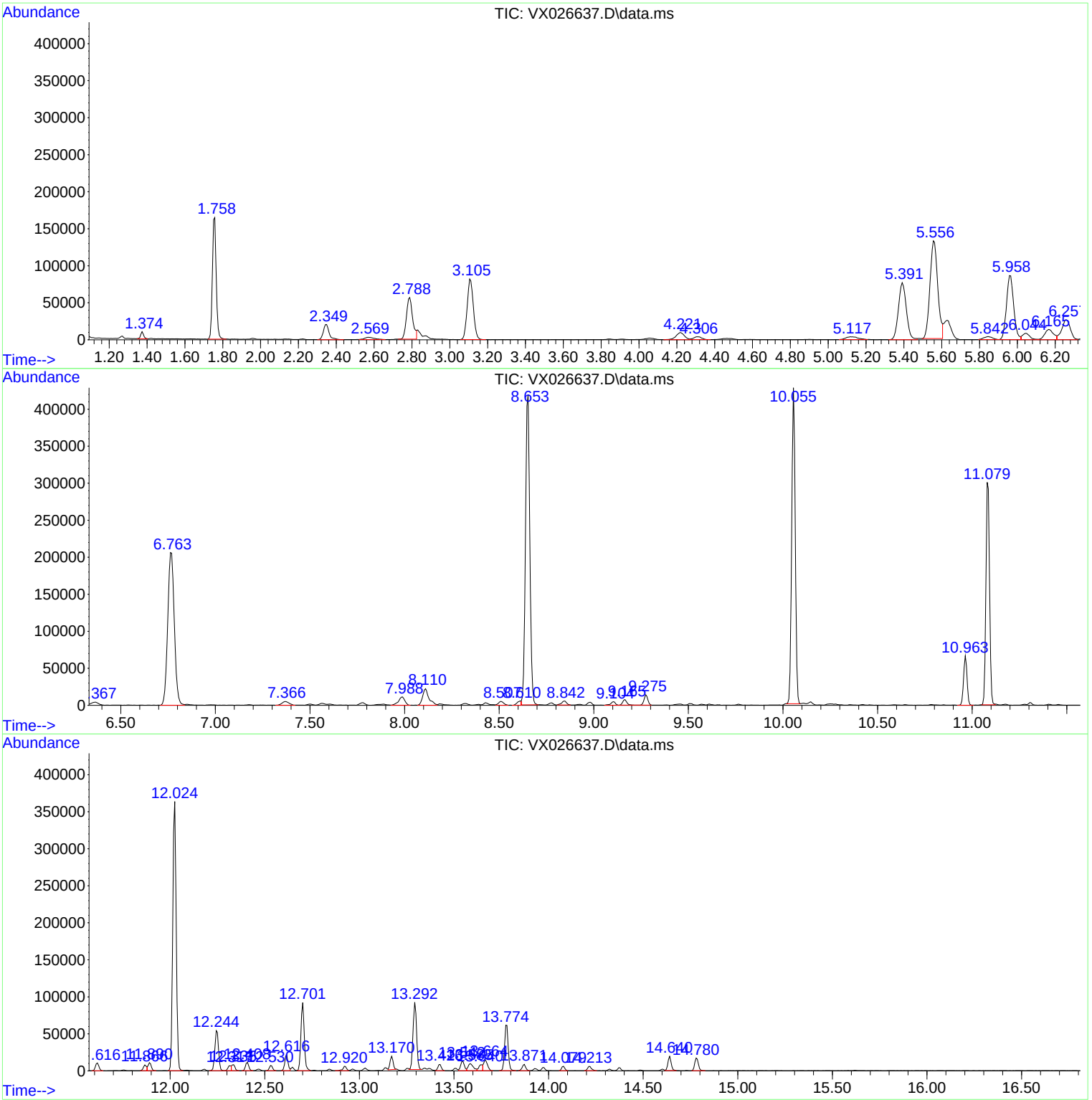
Sum of corrected areas: 5146545

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

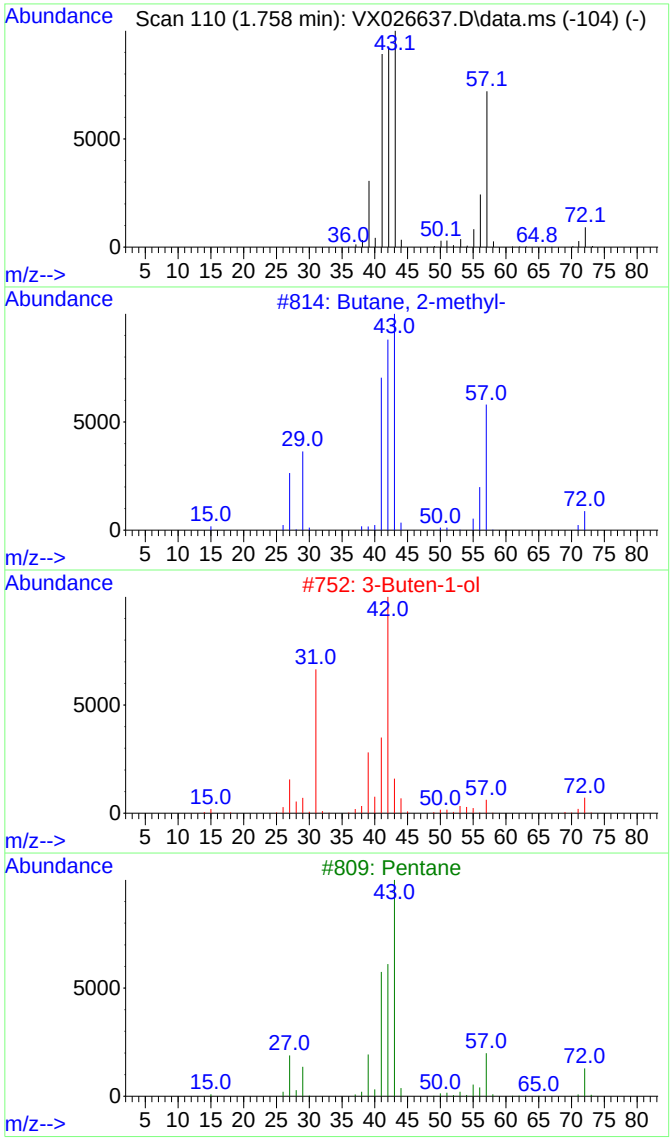
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

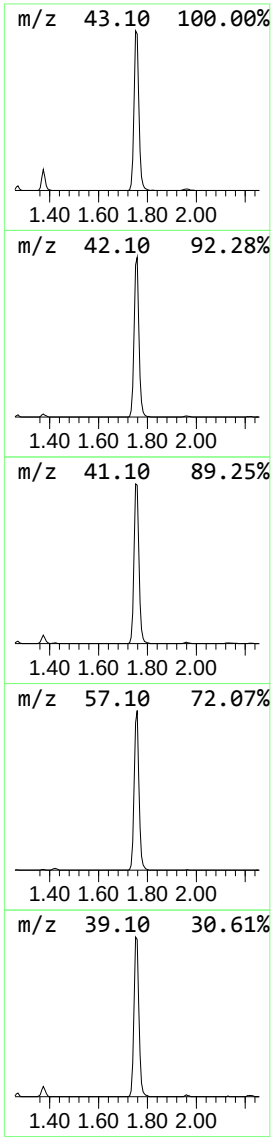
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.758	30.19 ug/l	229221	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	37
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5	Methane, isocyanato-	57	C2H3NO	000624-83-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

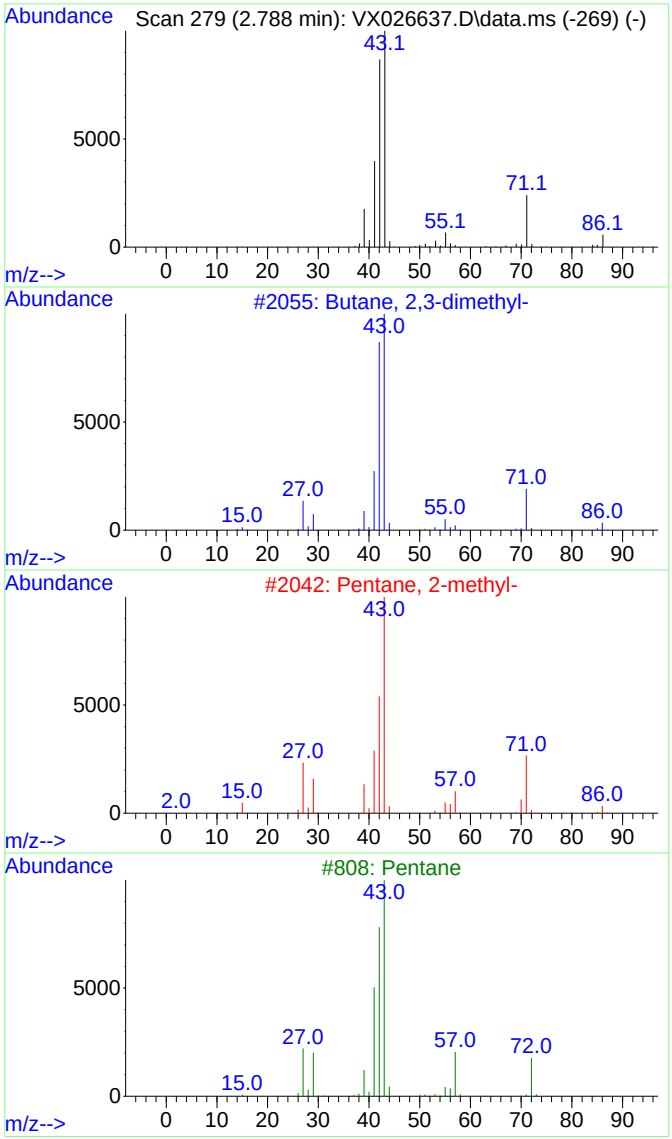
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

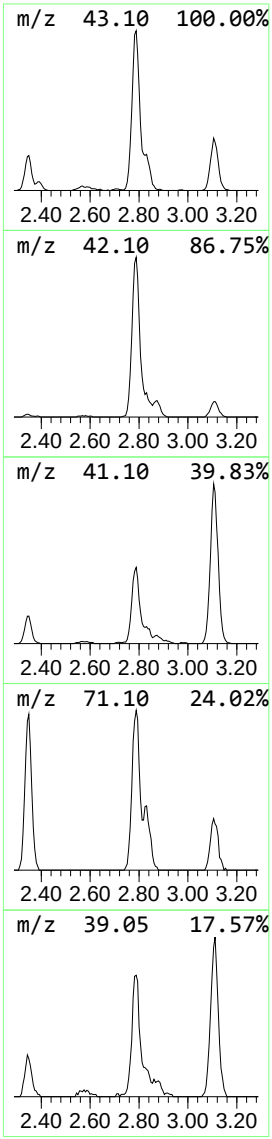
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.788	17.02 ug/l	129253	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3	Pentane	72	C5H12	000109-66-0	38
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	28
5	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

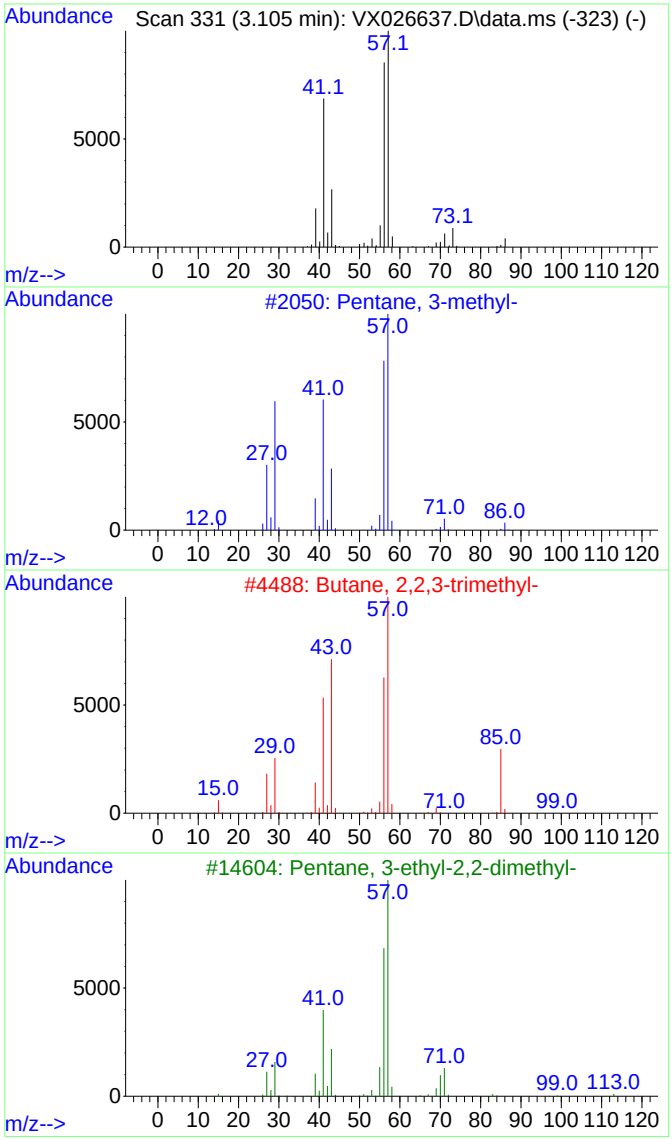
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

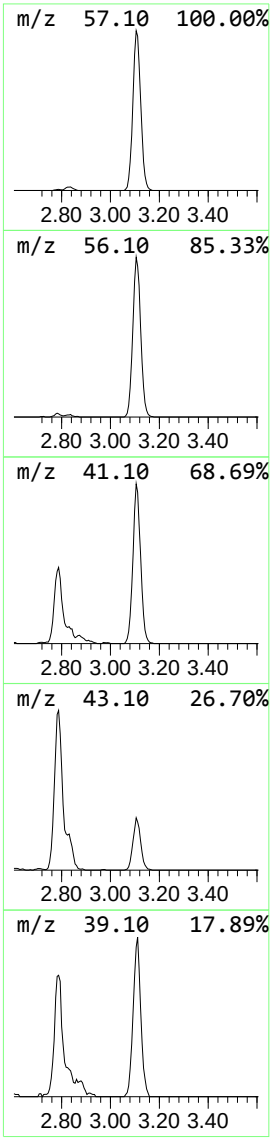
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	24.36 ug/l	184932	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

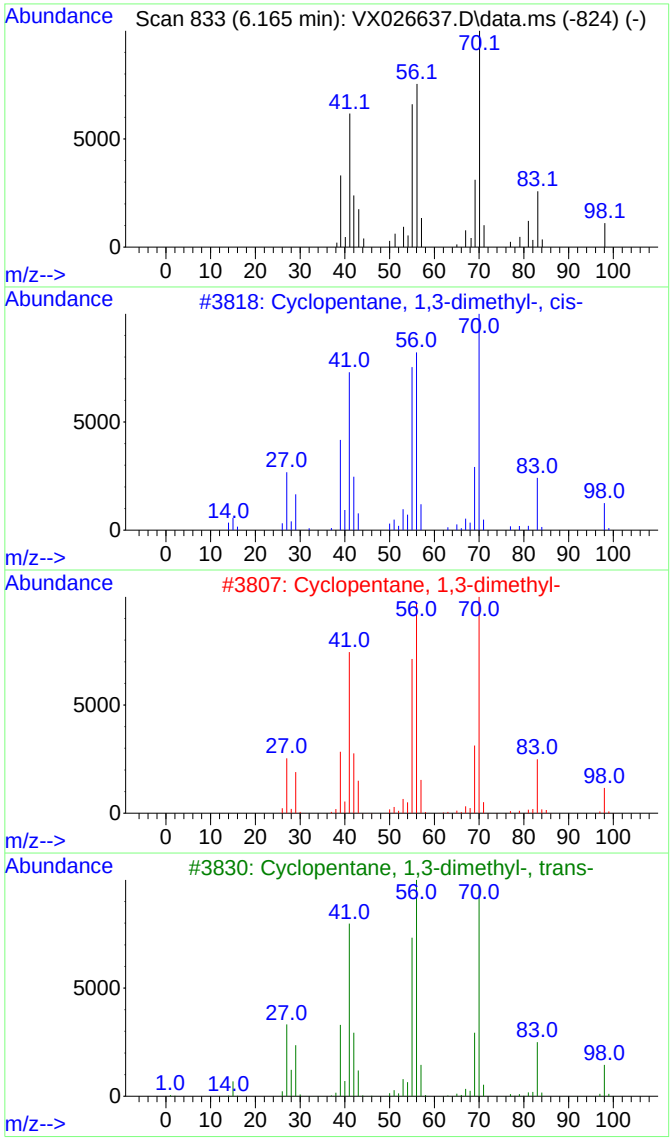
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

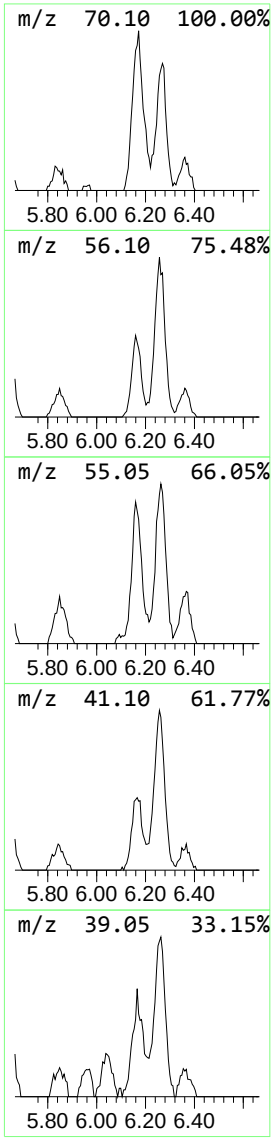
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, 1,3-dimethyl-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.165	5.90 ug/l	44780	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	94
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	93
3	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	90
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	87
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

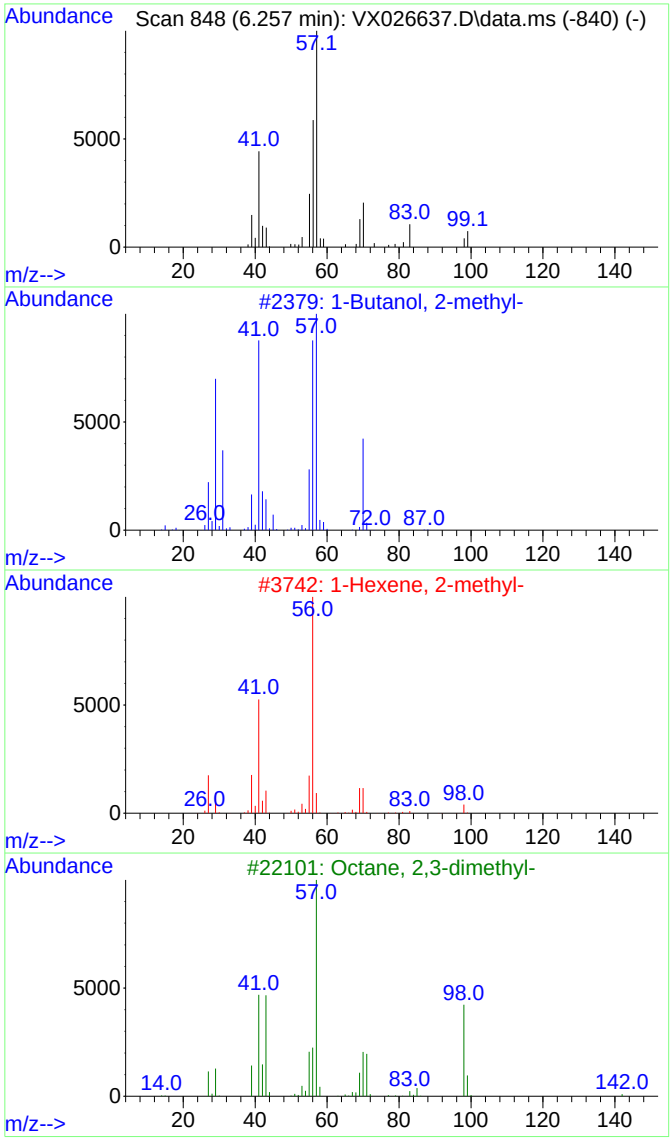
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

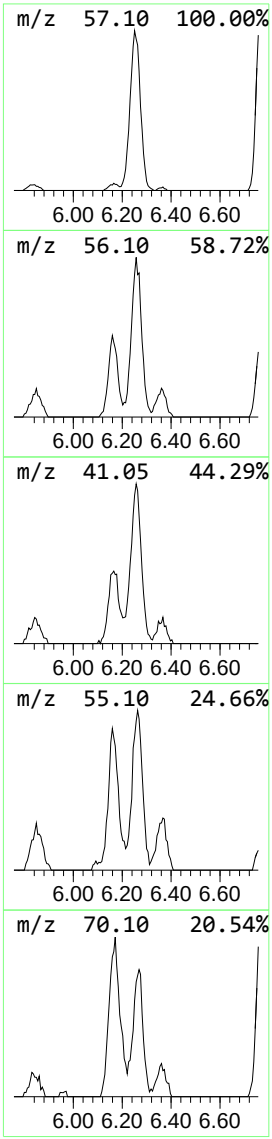
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	8.49 ug/l	83803	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	50
2	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	43
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	43
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	38
5	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

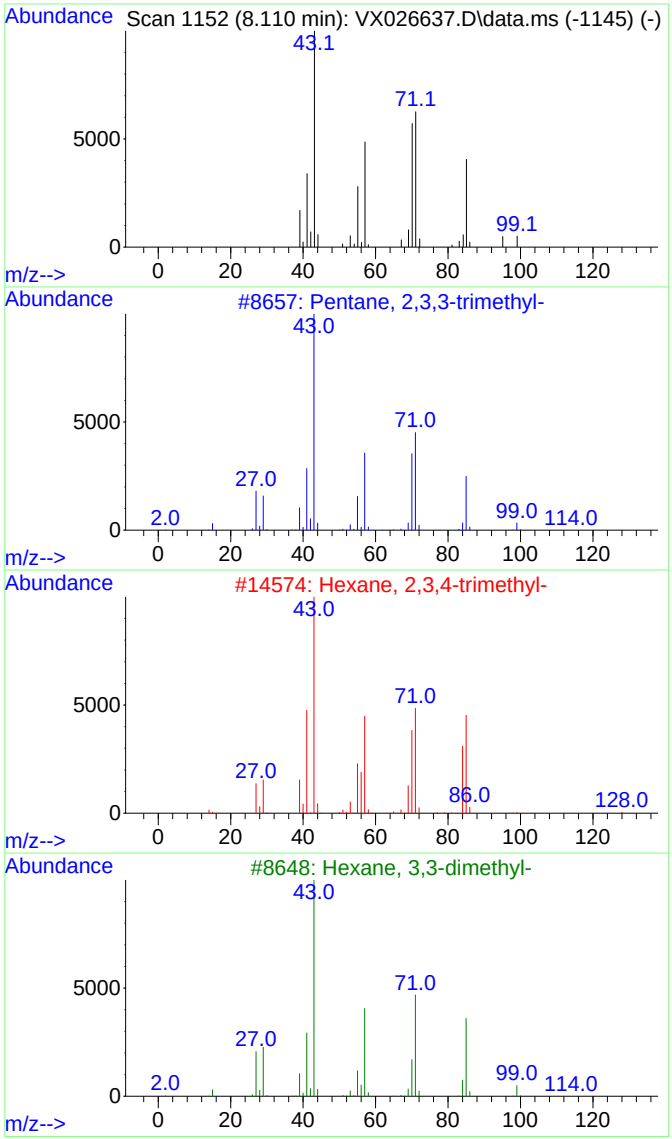
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

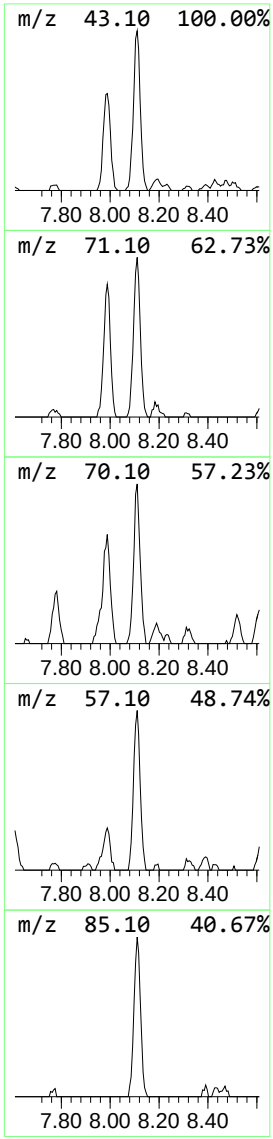
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	5.11 ug/l	50408	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	78
3	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

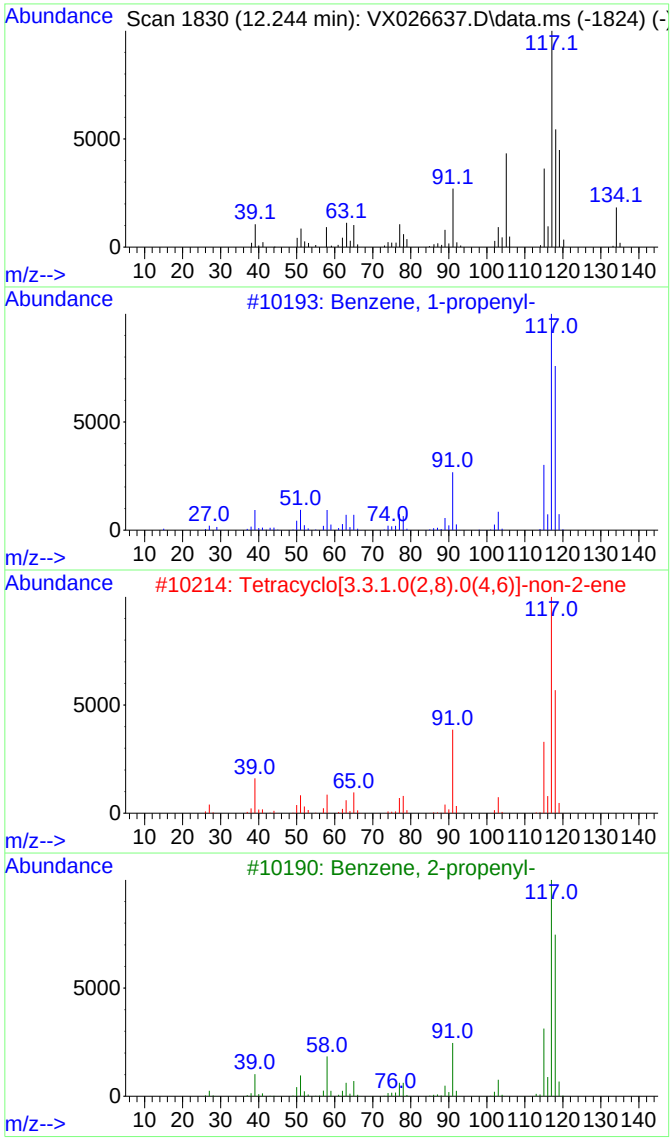
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

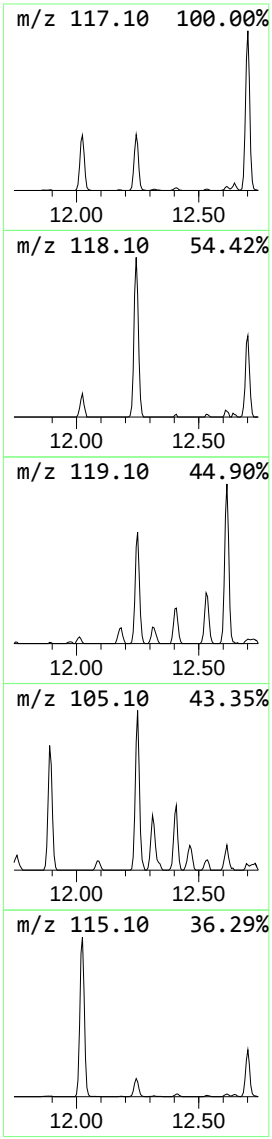
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-propenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	7.87 ug/l	72064	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-propenyl-	118	C9H10	000637-50-3	90
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	60
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
4	7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	60
5	Benzene, cyclopropyl-	118	C9H10	000873-49-4	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

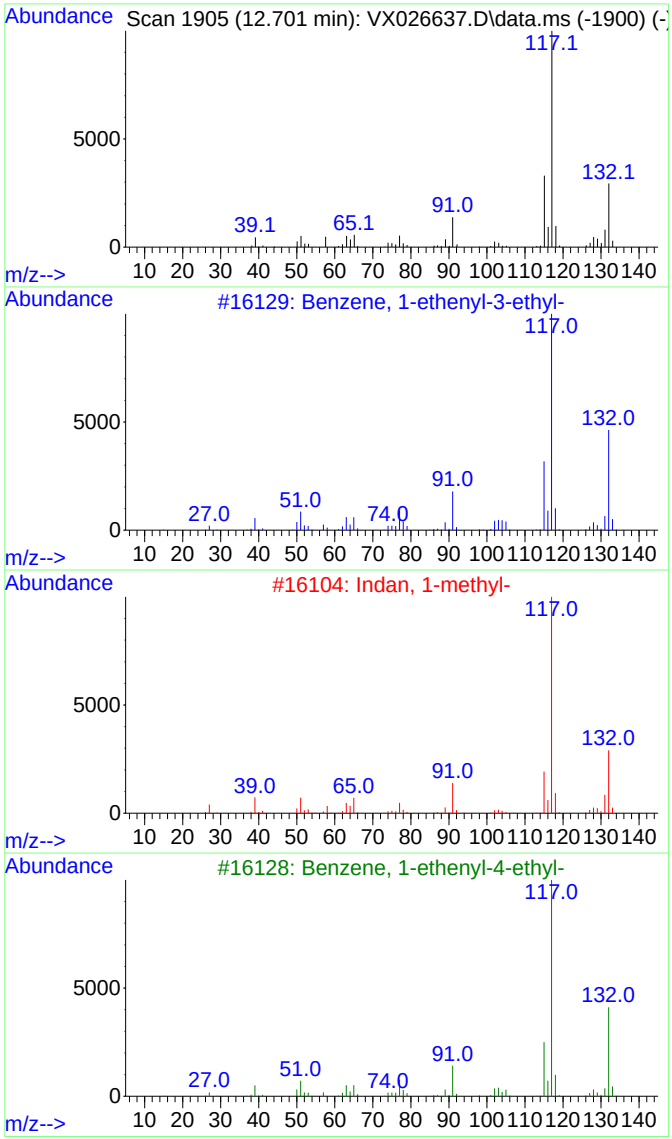
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

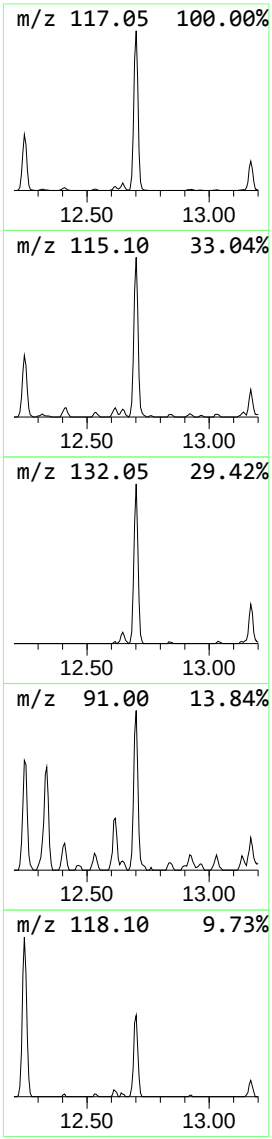
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	12.27 ug/l	112367	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	90
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

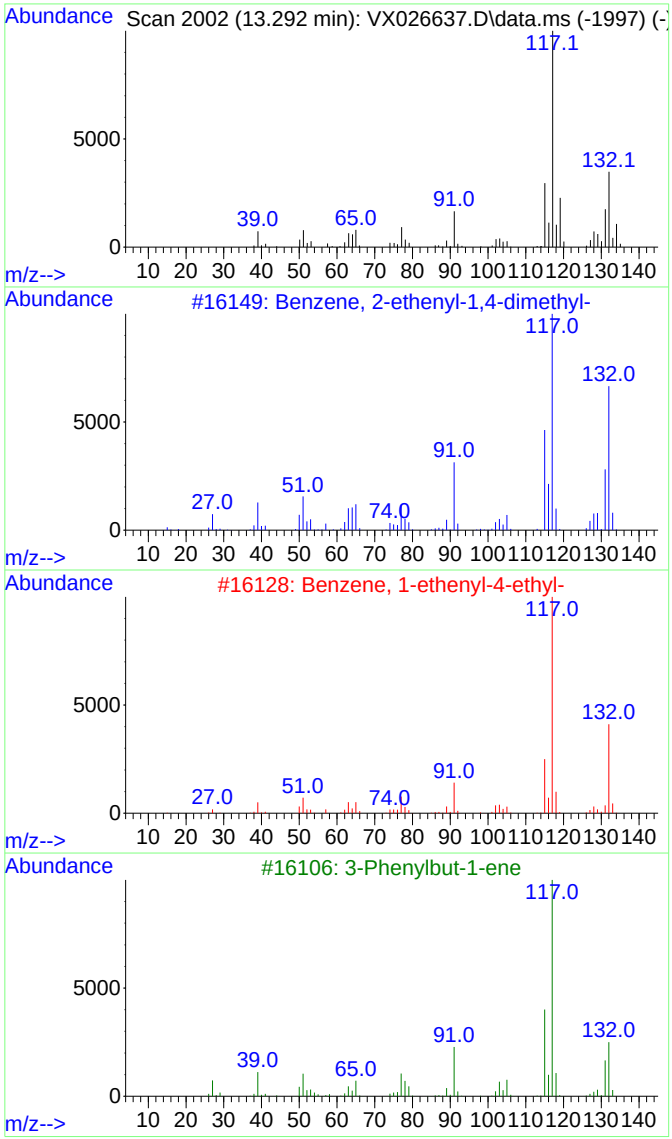
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

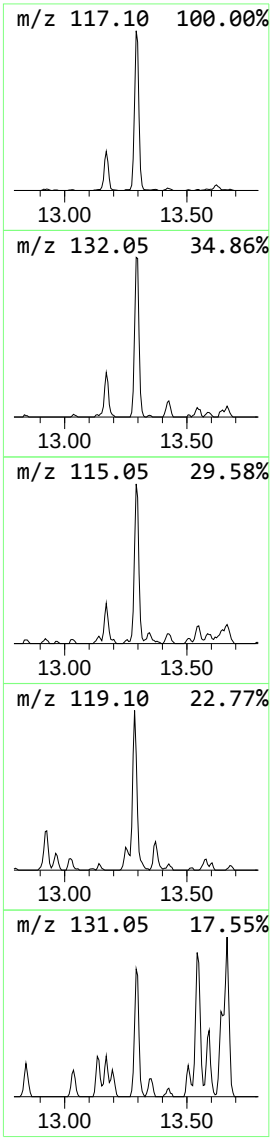
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	12.73 ug/l	116572	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	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
5	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012722\
Data File : VX026637.D
Acq On : 27 Jan 2022 20:07
Operator : JC/MD
Sample : N1297-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-14DA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
Butane, 2-methyl-	1.758	30.2	ug/l	229221	1	5.562	379655	50.0
Butane, 2,3-dim...	2.788	17.0	ug/l	129253	1	5.562	379655	50.0
Pentane, 3-methyl-	3.105	24.4	ug/l	184932	1	5.562	379655	50.0
Cyclopentane, 1...	6.165	5.9	ug/l	44780	1	5.562	379655	50.0
1-Butanol, 2-me...	6.257	8.5	ug/l	83803	2	6.769	493542	50.0
Pentane, 2,3,3-...	8.110	5.1	ug/l	50408	2	6.769	493542	50.0
Benzene, 1-prop...	12.244	7.9	ug/l	72064	4	12.024	457741	50.0
Benzene, 1-ethe...	12.701	12.3	ug/l	112367	4	12.024	457741	50.0
Benzene, 2-ethe...	13.292	12.7	ug/l	116572	4	12.024	457741	50.0