LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X062323W.M
Title : SW846 8260

Signal : TIC: VX036321.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	41	46	53	rVV	173829	193838	4.05%	0.454%
2	1.752	104	109	121	rVB	365948	482181	10.07%	1.128%
3	1.910	130	135	138	rBV	39692	53436	1.12%	0.125%
4	1.959	138	143	152	rVB	123037	188042	3.93%	0.440%
5	2.069	155	161	167	rBV	69960	98533	2.06%	0.231%
6	2.392	209	214	225	rVB	58103	123734	2.58%	0.290%
7	2.782	260	278	281	rBV4	21596	77020	1.61%	0.180%
8	2.825	281	285	288	rVV2	45360	91825	1.92%	0.215%
9	2.867	288	292	306	rVB	110885	233544	4.88%	0.547%
10	3.105	322	331	343	rVB2	53545	125541	2.62%	0.294%
11	4.306	518	528	541	rVB2	112520	321996	6.72%	0.753%
12	4.568	563	571	584	rBV2	16639	53820	1.12%	0.126%
13	5.385	692	705	713	rBV2	133550	397859	8.31%	0.931%
14	5.477	713	720	725	rVV2	58801	183654	3.83%	0.430%
15	5.550	725	732	753	rVB	197239	591977	12.36%	1.385%
16	5.958	789	799	804	rBV	164465	429299	8.96%	1.005%
17	6.038	804	812	827	rVB	1823109	4788906	100.00%	11.206%
18	6.361	856	865	880	rVB9	13948	50587	1.06%	0.118%
19	6.763	922	931	943	rBV	348415	830084	17.33%	1.942%
20	7.379	1021	1032	1041	rBV4	52899	139728	2.92%	0.327%
21	8.647	1234	1240	1246	rBV	755102	1145073	23.91%	2.680%
22	8.720	1246	1252	1261	rVB	1093416	1694510	35.38%	3.965%
23	8.958	1283	1291	1297	rBV	156284	245084	5.12%	0.574%
24	9.049	1297	1306	1312	rVV	174781	275376	5.75%	0.644%
25	10.055	1461	1471	1483	rBV	751569	1072357	22.39%	2.509%
26	10.195	1488	1494	1500	rBV	3774665	4740708	98.99%	11.094%
27	10.305	1506	1512	1519	rVB	1545294	1987199	41.50%	4.650%
28	10.640	1561	1567	1577	rVB	3312547	4147767	86.61%	9.706%
29	10.963	1613	1620	1625	rBV	134563	178544	3.73%	0.418%
30	11.079	1634	1639	1645	rBV	611828	764698	15.97%	1.789%
31	11.305	1671	1676	1683	rVB	200792	257892	5.39%	0.603%
32	11.396	1683	1691	1696	rVV	465645	630731	13.17%	1.476%
33	11.451	1696	1700	1705	rVB	428039	508764	10.62%	1.191%
34	11.610	1721	1726	1733	rBV	2379118	2858189	59.68%	6.688%
35	11.750	1744	1749	1755	rVB	1113307	1326326	27.70%	3.104%
36	11.969	1780	1785	1789	rBV2	36339	51674	1.08%	0.121%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X062323W.M
Title : SW846 8260

37	12.018	1789	1793	1799	rVV	754603	919895	19.21%	2.153%
38	12.085	1799	1804	1812	rVB	2673101	3073269	64.17%	7.192%
39	12.244	1823	1830	1837	rBV	2831870	3605072	75.28%	8.436%
40	12.317	1837	1842	1850	rVB2	146379	230226	4.81%	0.539%
41	12.408	1852	1857	1861	rBV2	52588	72399	1.51%	0.169%
42	12.463	1861	1866	1871	rVB	105069	132974	2.78%	0.311%
43	12.530	1872	1877	1886	rBV	126495	191878	4.01%	0.449%
44	12.610	1886	1890	1893	rBV	238003	280805	5.86%	0.657%
45	12.646	1893	1896	1900	rVV	92841	109882	2.29%	0.257%
46	12.695	1900	1904	1912	rVV2	386880	532352	11.12%	1.246%
47	12.847	1924	1929	1935	rVB	150589	186608	3.90%	0.437%
48	12.920	1935	1941	1944	rBV	94251	122895	2.57%	0.288%
49	12.963	1944	1948	1954	rVB2	57265	81749	1.71%	0.191%
50	13.170	1978	1982	1991	rVB	94057	133387	2.79%	0.312%
51	13.292	1997	2002	2007	rVB2	526744	645295	13.47%	1.510%
52	13.420	2019	2023	2028	rVB	80043	95830	2.00%	0.224%
53	13.774	2075	2081	2085	rBV	429730	532556	11.12%	1.246%
54	13.823	2085	2089	2092	rVV	66719	93222	1.95%	0.218%
55	13.865	2092	2096	2102	rVB	161464	207376	4.33%	0.485%
56	14.780	2241	2246	2251	rBV	114017	145749	3.04%	0.341%

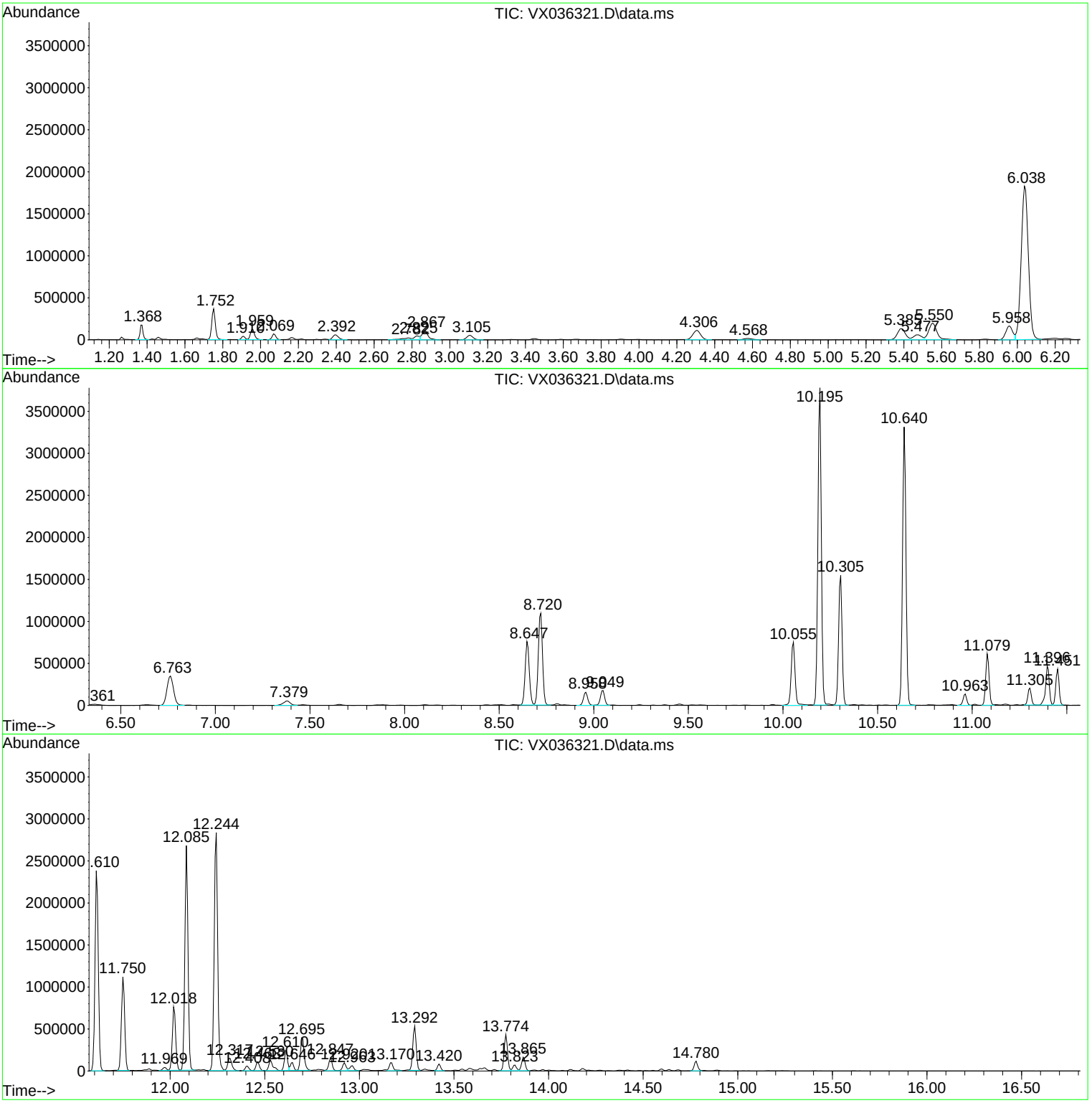
Sum of corrected areas: 42733915

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

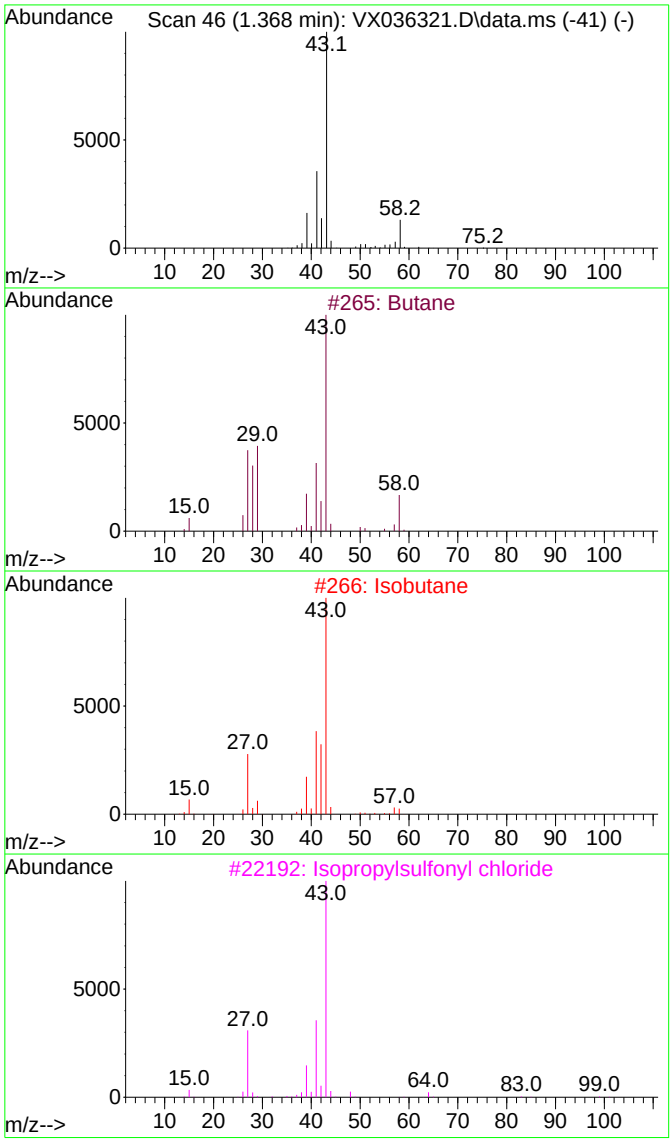
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

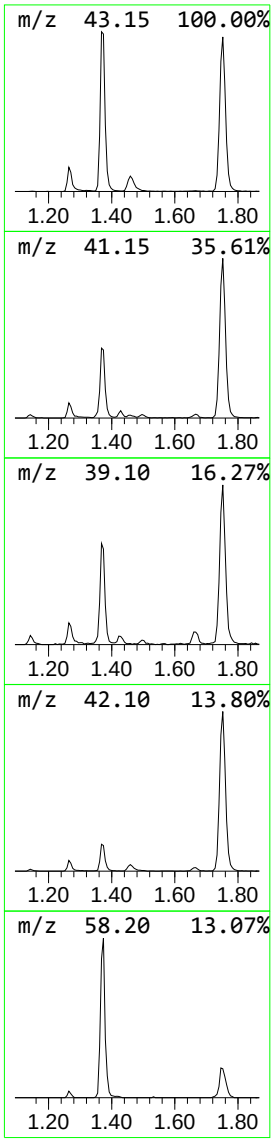
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.368	16.37 ug/l	193838	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

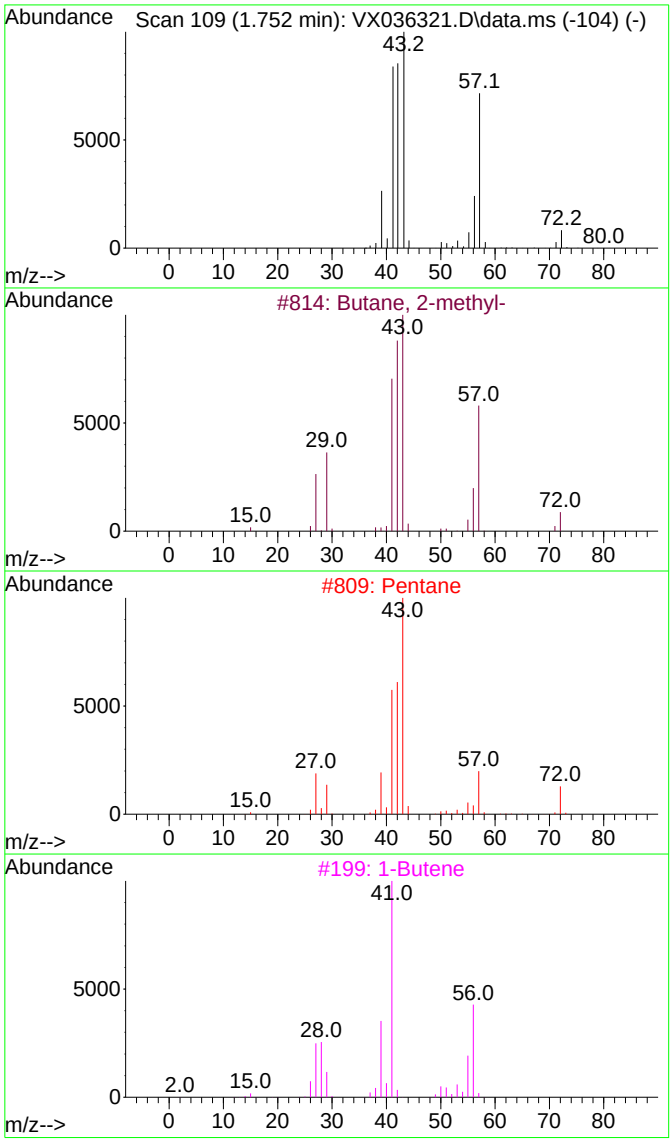
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

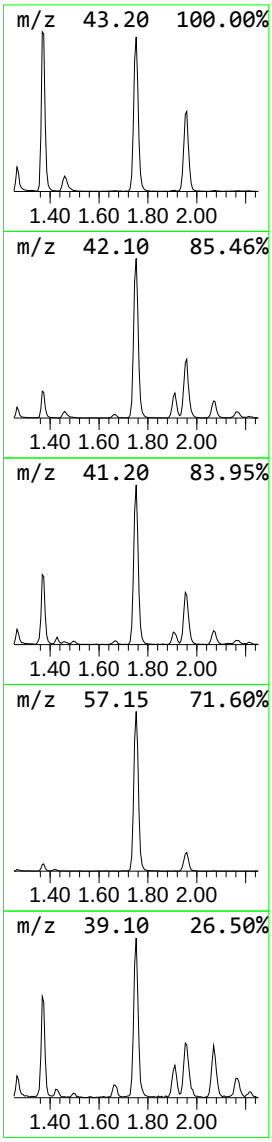
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	40.73 ug/l	482181	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Pentane	72	C5H12	000109-66-0	39
3	1-Butene	56	C4H8	000106-98-9	10
4	3-Buten-1-ol	72	C4H8O	000627-27-0	9
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

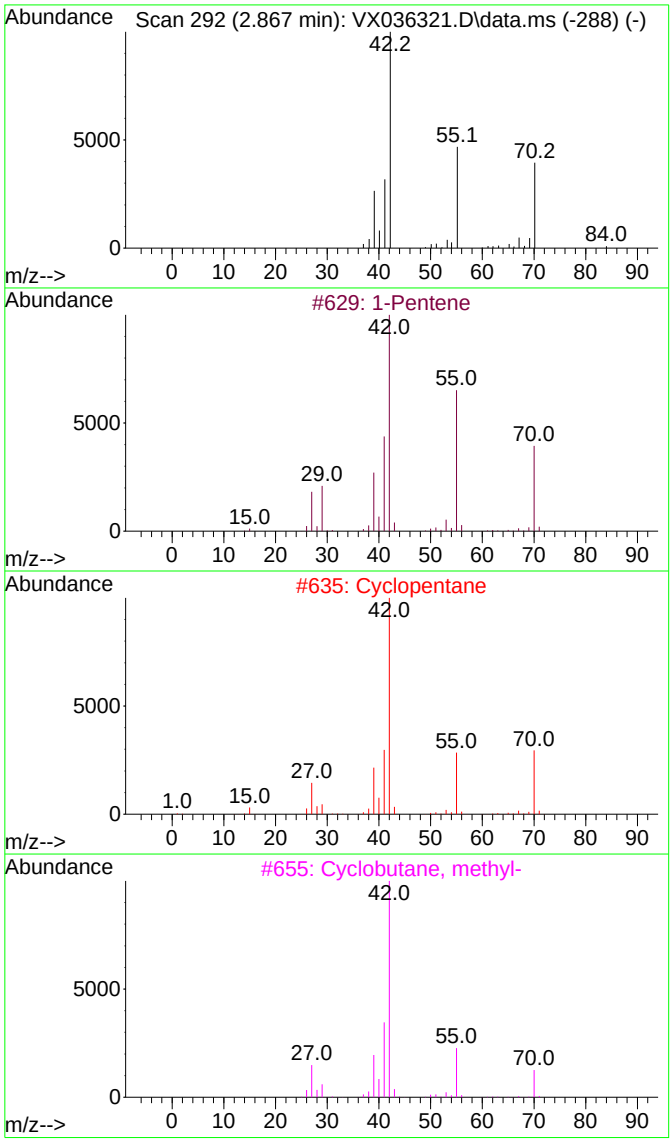
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

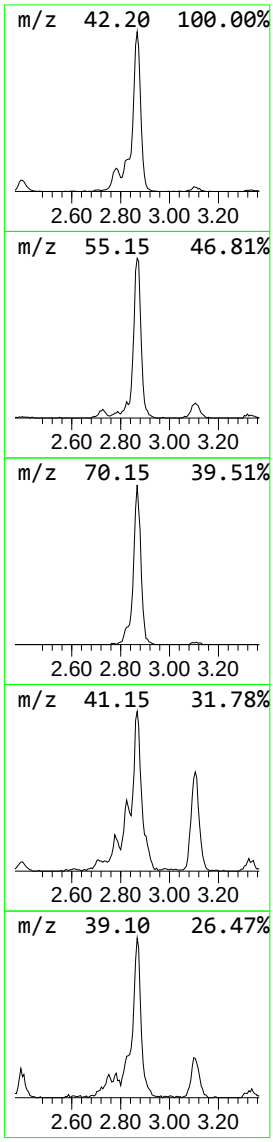
****

Peak Number 3 1-Pentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	19.73 ug/l	233544	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclopentane	70	C5H10	000287-92-3	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	3-Buten-1-ol	72	C4H8O	000627-27-0	38
5	Cyclobutanone	70	C4H6O	001191-95-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

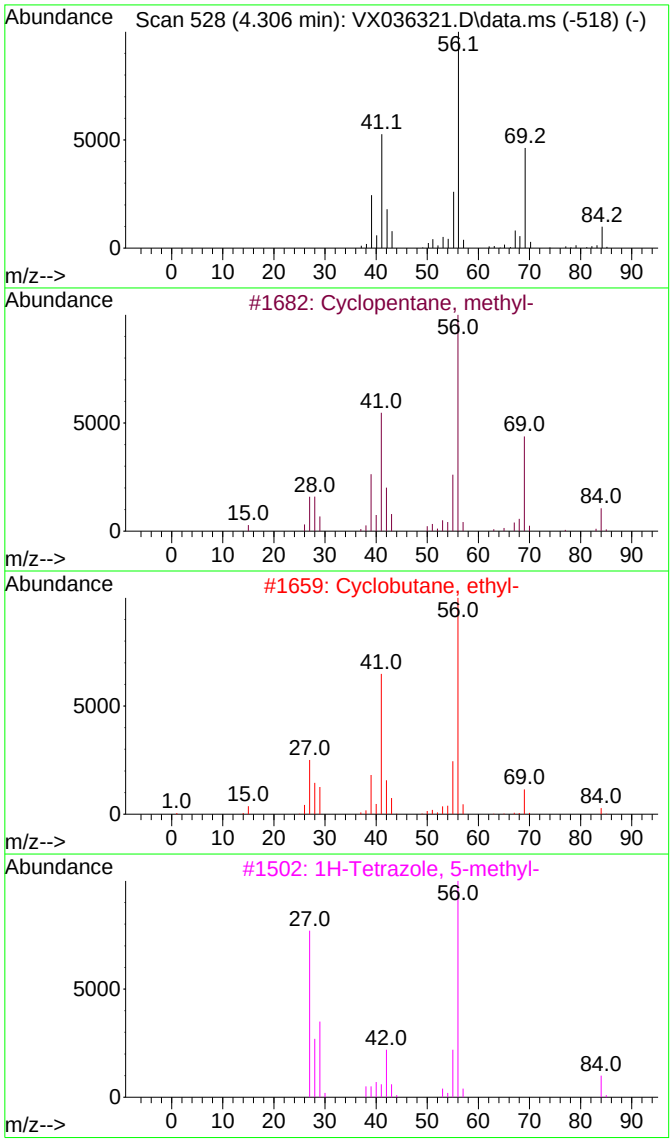
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

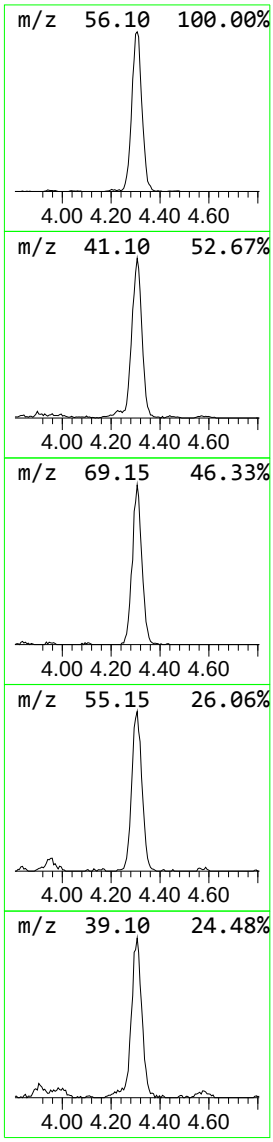
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	27.20 ug/l	321996	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53
5	Cyclobutane	56	C4H8	000287-23-0	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

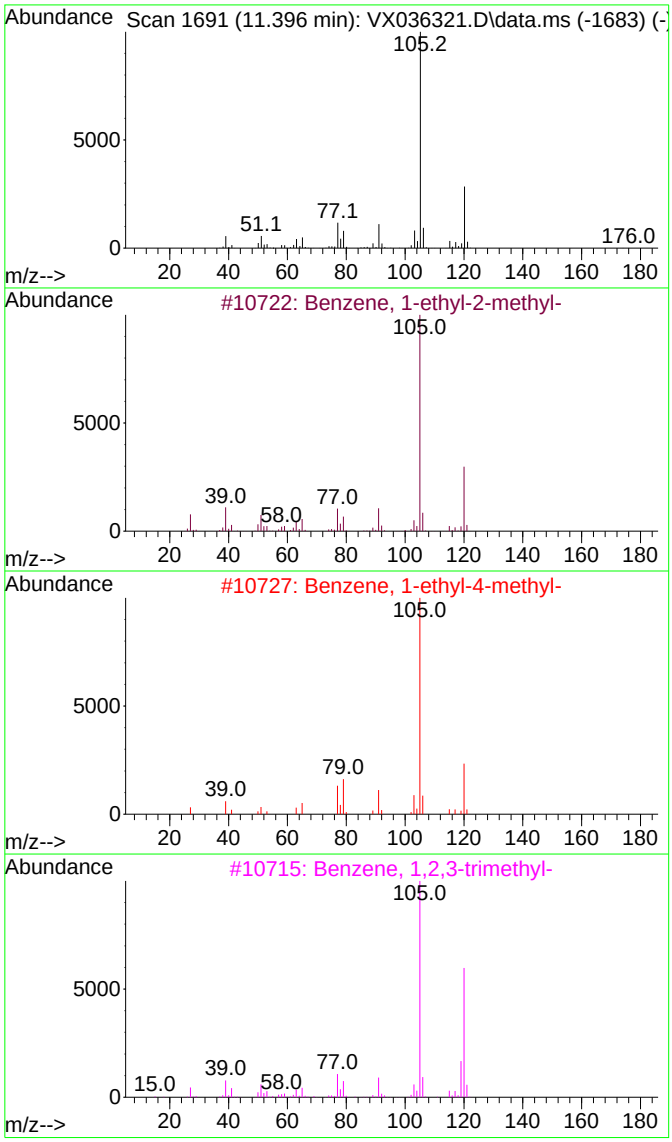
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

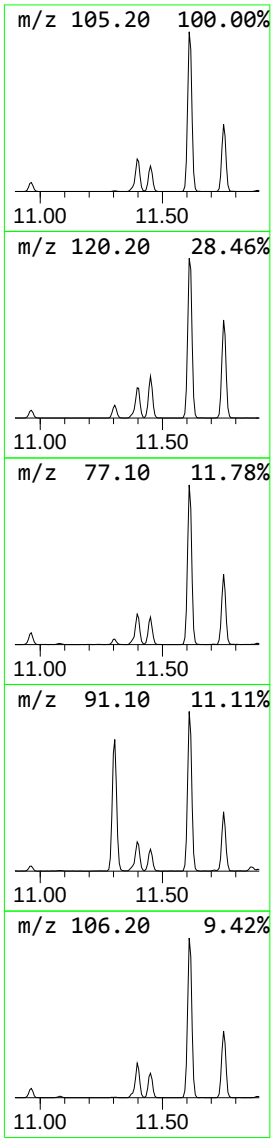
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.396	34.28 ug/l	630731	1,4-Dichlorobenzene-d4	12.018

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	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

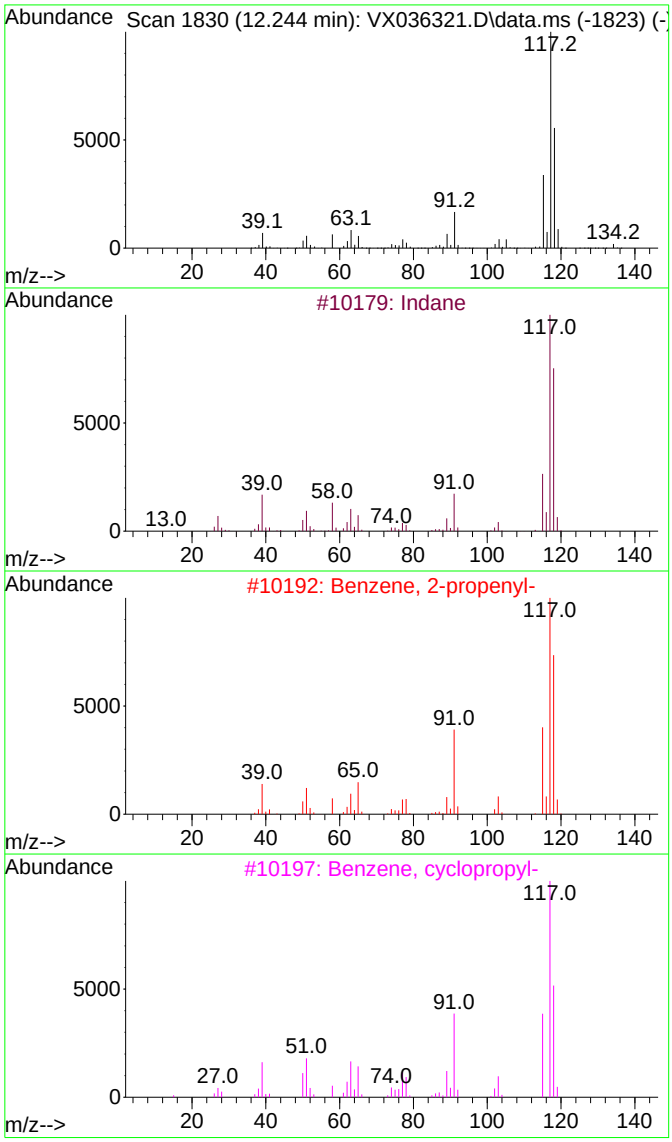
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

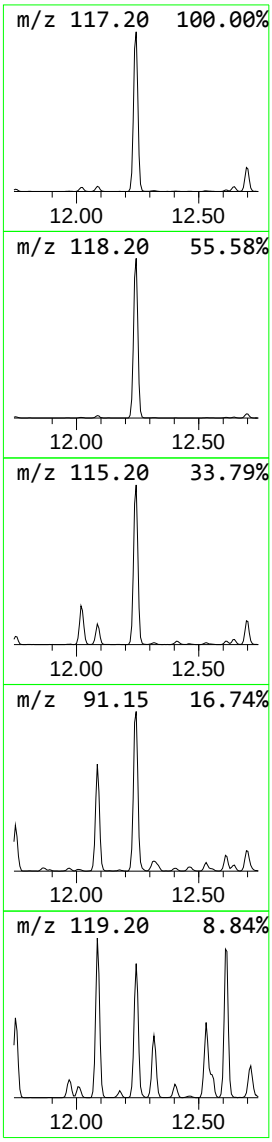
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	195.95 ug/l	3605070	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

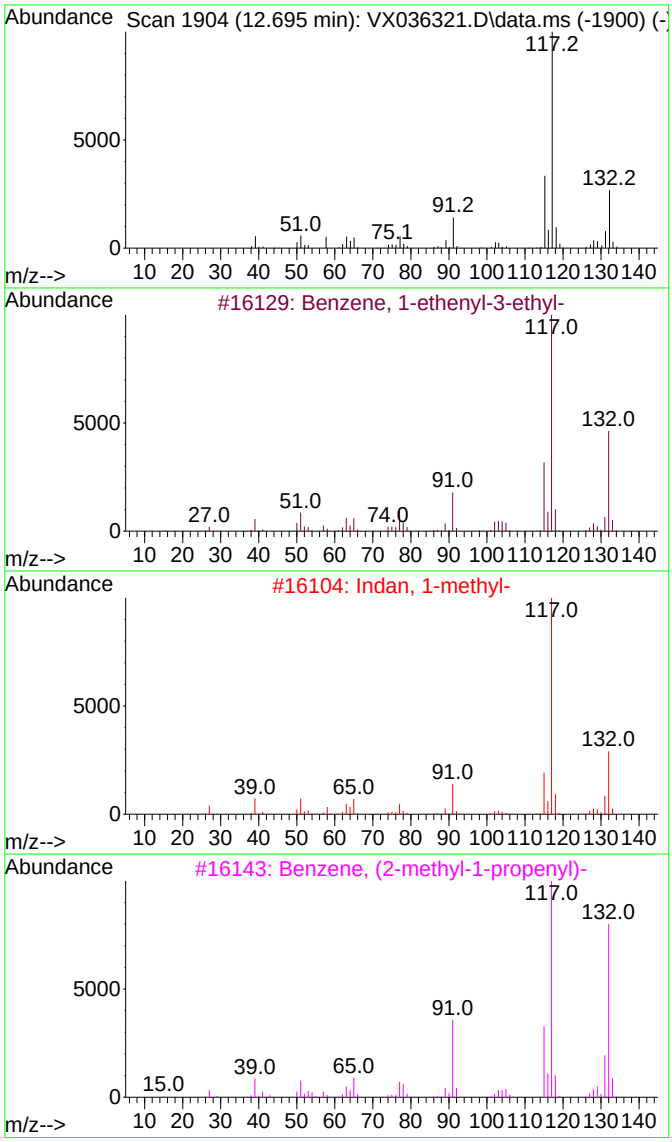
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

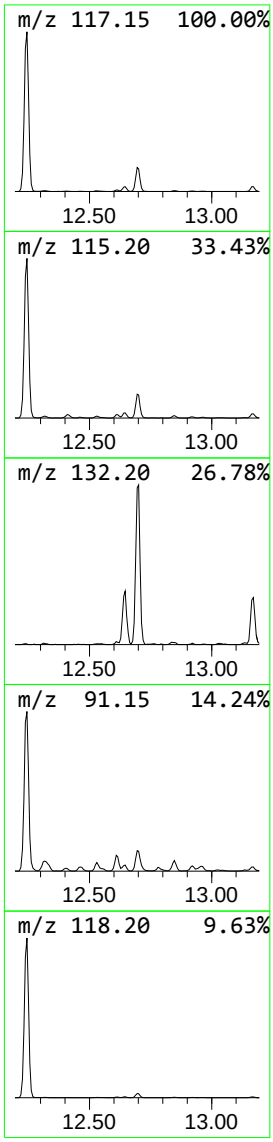
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	28.94 ug/l	532352	1,4-Dichlorobenzene-d4	12.018

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, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

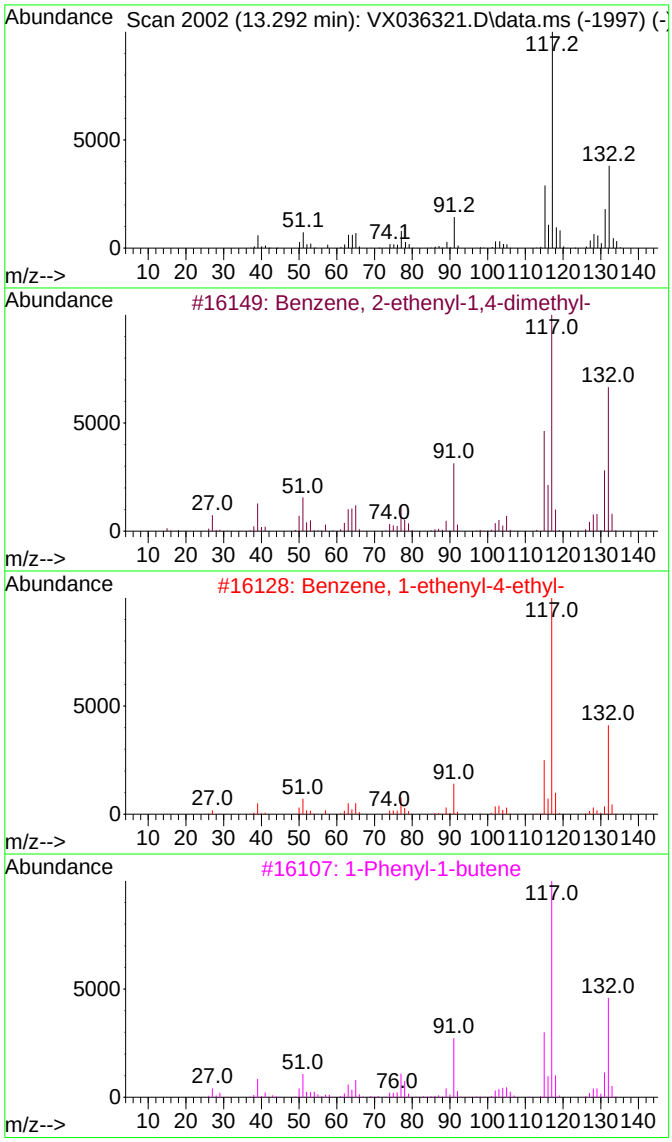
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.M
Quant Title : SW846 8260

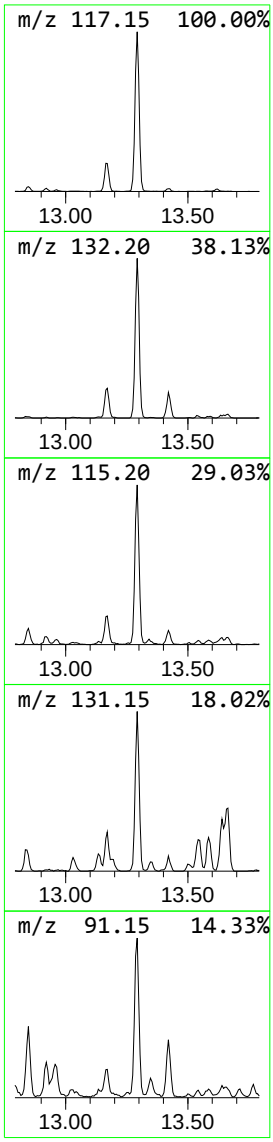
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	35.07 ug/l	645295	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	96
2	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	93
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	91
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062423\
Data File : VX036321.D
Acq On : 24 Jun 2023 18:58
Operator : JC/MD
Sample : 03339-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062323W.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	1.368	16.4	ug/l	193838	1	5.556	591977	50.0
Butane, 2-methyl-	1.752	40.7	ug/l	482181	1	5.556	591977	50.0
1-Pentene	2.867	19.7	ug/l	233544	1	5.556	591977	50.0
Cyclopentane, m...	4.306	27.2	ug/l	321996	1	5.556	591977	50.0
Benzene, 1-ethy...	11.396	34.3	ug/l	630731	4	12.018	919895	50.0
Indane	12.244	195.9	ug/l	3605070	4	12.018	919895	50.0
Benzene, 1-ethe...	12.695	28.9	ug/l	532352	4	12.018	919895	50.0
Benzene, 2-ethe...	13.292	35.1	ug/l	645295	4	12.018	919895	50.0