LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X062321W.M
Title : SW846 8260

Signal : TIC: VX023008.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	37	rVB2	12683	20849	2.35%	0.304%
2	1.752	104	109	118	rVB	29329	42489	4.79%	0.620%
3	1.959	137	143	148	rVB	6897	10381	1.17%	0.151%
4	2.782	268	278	281	rBV2	11980	25268	2.85%	0.369%
5	2.825	281	285	290	rVV	21209	46219	5.21%	0.674%
6	2.867	290	292	302	rVV4	7771	16935	1.91%	0.247%
7	3.105	324	331	345	rVB3	26940	67556	7.61%	0.985%
8	3.453	381	388	394	rVB3	4503	9713	1.09%	0.142%
9	3.739	426	435	444	rVB4	6166	15148	1.71%	0.221%
10	3.843	444	452	459	rBV3	3810	9697	1.09%	0.141%
11	4.306	520	528	539	rVB2	22419	62322	7.02%	0.909%
12	5.190	663	673	684	rVB8	4257	14971	1.69%	0.218%
13	5.397	696	707	715	rBV2	41533	121951	13.74%	1.779%
14	5.483	715	721	726	rVV5	6435	18321	2.06%	0.267%
15	5.562	726	734	743	rVB	64433	173393	19.54%	2.529%
16	5.836	767	779	790	rBV5	7837	25547	2.88%	0.373%
17	5.970	790	801	807	rBV2	56306	151684	17.09%	2.213%
18	6.050	807	814	825	rVV	62179	166666	18.78%	2.431%
19	6.172	825	834	843	rVV7	8357	36408	4.10%	0.531%
20	6.257	843	848	855	rVV4	11741	34283	3.86%	0.500%
21	6.342	855	862	875	rVB5	15612	56047	6.31%	0.818%
22	6.769	921	932	940	rBV	126633	297615	33.53%	4.341%
23	6.848	942	945	956	rVB4	11748	29637	3.34%	0.432%
24	7.178	991	999	1006	rVB3	6590	14640	1.65%	0.214%
25	7.379	1019	1032	1043	rBV4	20675	56366	6.35%	0.822%
26	7.659	1073	1078	1086	rBV3	4735	9053	1.02%	0.132%
27	7.988	1123	1132	1142	rVB7	4989	14637	1.65%	0.214%
28	8.110	1144	1152	1154	rBV3	8278	14211	1.60%	0.207%
29	8.147	1154	1158	1163	rVB	9201	16068	1.81%	0.234%
30	8.507	1212	1217	1226	rVB4	13645	29762	3.35%	0.434%
31	8.610	1226	1234	1235	rBV2	5577	9350	1.05%	0.136%
32	8.653	1235	1241	1248	rVB	256766	402401	45.34%	5.870%
33	8.720	1248	1252	1258	rBV	11993	18652	2.10%	0.272%
34	9.165	1320	1325	1329	rBV2	8792	13064	1.47%	0.191%
35	10.055	1466	1471	1477	rBV	246786	330984	37.29%	4.828%
36	10.195	1489	1494	1500	rVB	196460	253753	28.59%	3.702%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

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\82X062321W.M
Title : SW846 8260

37	10.305	1505	1512	1519	rVB	654854	887550	100.00%	12.947%
38	10.646	1562	1568	1578	rBV	87815	114719	12.93%	1.673%
39	10.963	1614	1620	1627	rVB	31551	39723	4.48%	0.579%
40	11.085	1634	1640	1646	rBV	188310	240563	27.10%	3.509%
41	11.305	1672	1676	1683	rVB	52650	63625	7.17%	0.928%
42	11.384	1683	1689	1691	rBV	96270	141492	15.94%	2.064%
43	11.457	1696	1701	1707	rVB	79123	103462	11.66%	1.509%
44	11.616	1722	1727	1735	rVB	116035	141241	15.91%	2.060%
45	11.756	1744	1750	1756	rVB	380191	454227	51.18%	6.626%
46	12.024	1789	1794	1799	rBV	235566	289556	32.62%	4.224%
47	12.091	1799	1805	1810	rVB	177251	220444	24.84%	3.216%
48	12.244	1823	1830	1838	rBV	300070	383719	43.23%	5.598%
49	12.317	1838	1842	1849	rVB3	32144	48754	5.49%	0.711%
50	12.414	1852	1858	1862	rBV2	19449	26653	3.00%	0.389%
51	12.469	1862	1867	1873	rVB2	23374	32185	3.63%	0.470%
52	12.536	1873	1878	1880	rBV	22041	32282	3.64%	0.471%
53	12.555	1880	1881	1886	rVB	17453	16270	1.83%	0.237%
54	12.616	1886	1891	1894	rBV	80879	94703	10.67%	1.381%
55	12.646	1894	1896	1900	rVV	20118	22017	2.48%	0.321%
56	12.701	1900	1905	1912	rVB2	81039	110314	12.43%	1.609%
57	12.847	1924	1929	1934	rVB2	13718	18406	2.07%	0.268%
58	12.927	1936	1942	1945	rBV	54536	66738	7.52%	0.974%
59	12.963	1945	1948	1954	rVB	44199	51699	5.82%	0.754%
60	13.030	1954	1959	1965	rBV4	5020	10104	1.14%	0.147%
61	13.170	1978	1982	1988	rVB	54383	65876	7.42%	0.961%
62	13.292	1998	2002	2008	rVB2	114257	148426	16.72%	2.165%
63	13.426	2020	2024	2028	rVB2	20966	26395	2.97%	0.385%
64	13.548	2040	2044	2047	rVV	14099	19989	2.25%	0.292%
65	13.585	2047	2050	2056	rVV5	12922	22908	2.58%	0.334%
66	13.646	2056	2060	2061	rVV4	7168	9916	1.12%	0.145%
67	13.664	2061	2063	2069	rVB2	13508	18585	2.09%	0.271%
68	13.780	2075	2082	2088	rBV	160525	203119	22.89%	2.963%
69	14.079	2124	2131	2136	rBV	8320	10296	1.16%	0.150%
70	14.219	2149	2154	2164	rBV3	6795	12235	1.38%	0.178%
71	14.640	2218	2223	2233	rVB	29980	36682	4.13%	0.535%
72	14.780	2241	2246	2251	rVB	26324	34238	3.86%	0.499%

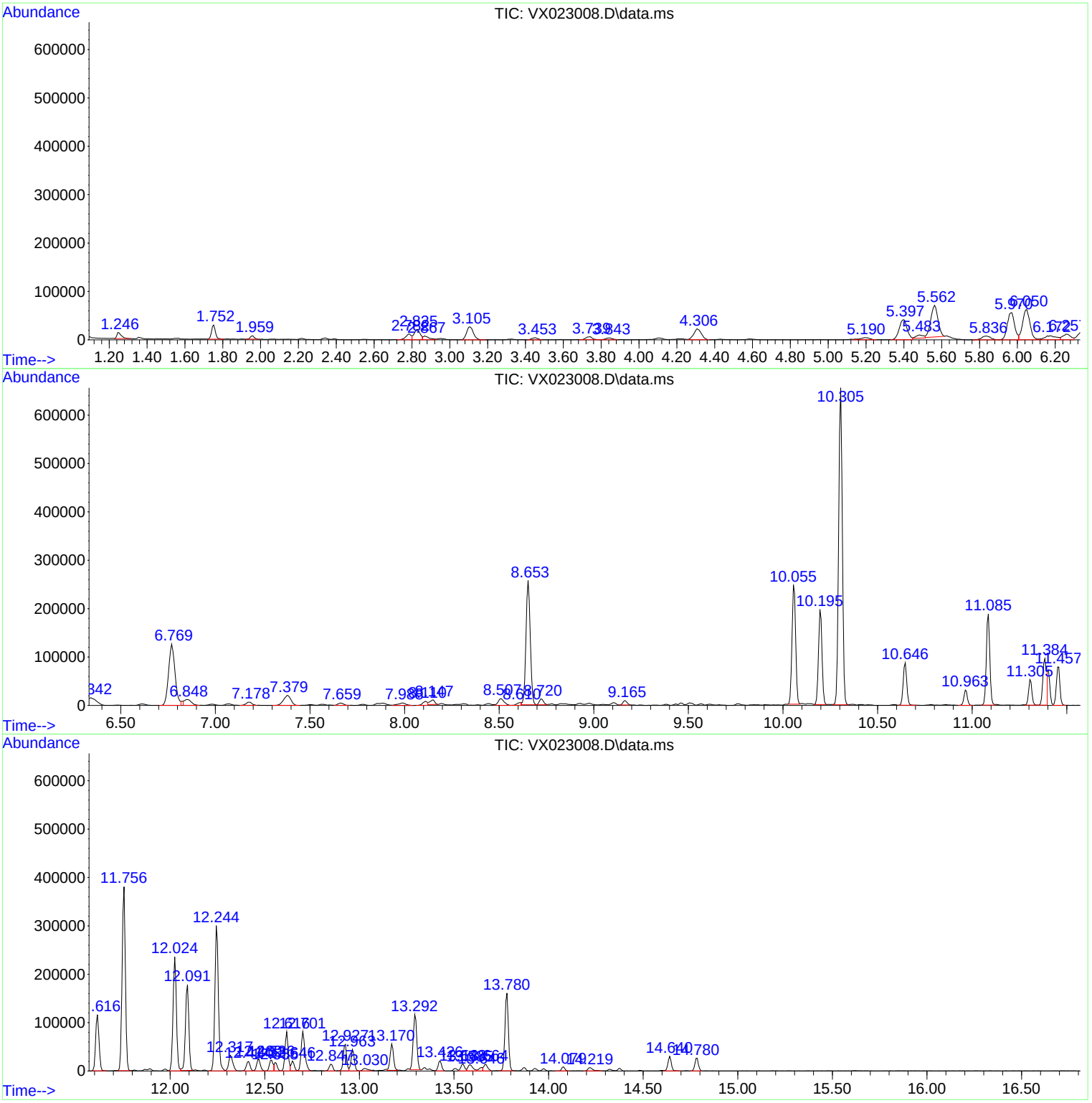
Sum of corrected areas: 6855152

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

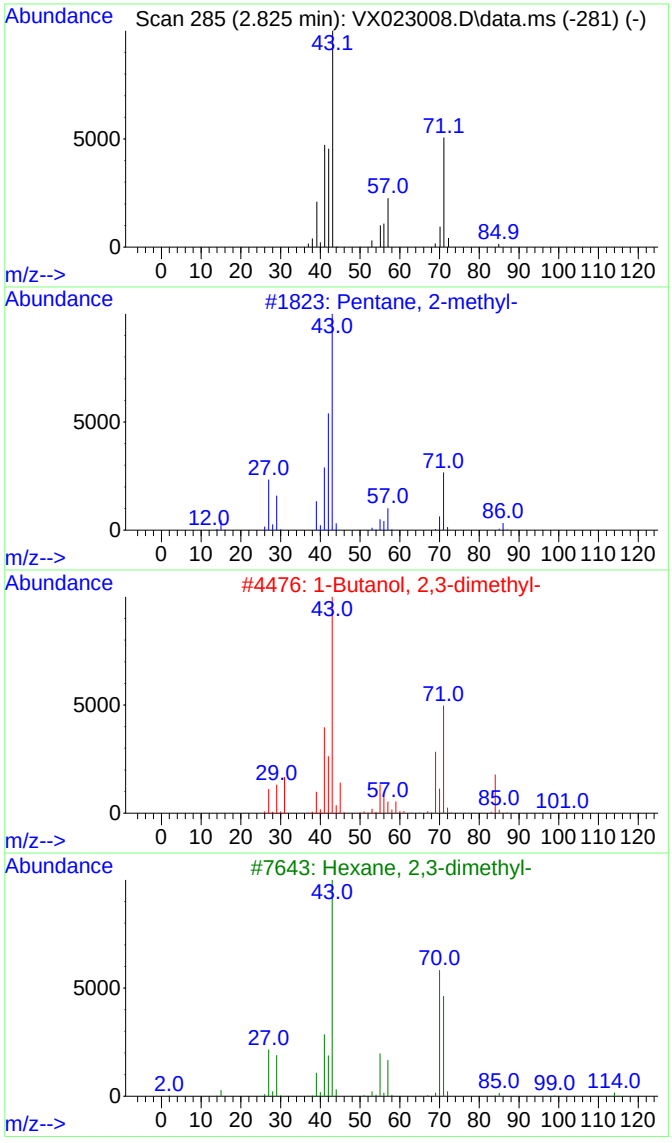
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

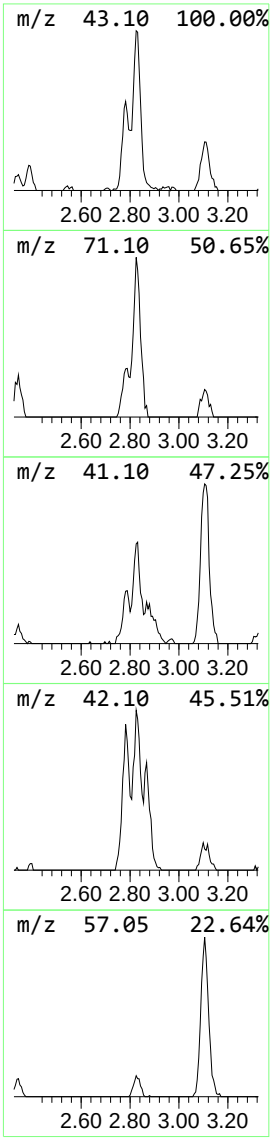
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Pentane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.825	13.33 ug/l	46219	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	74
2	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38
3	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
4	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	25
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

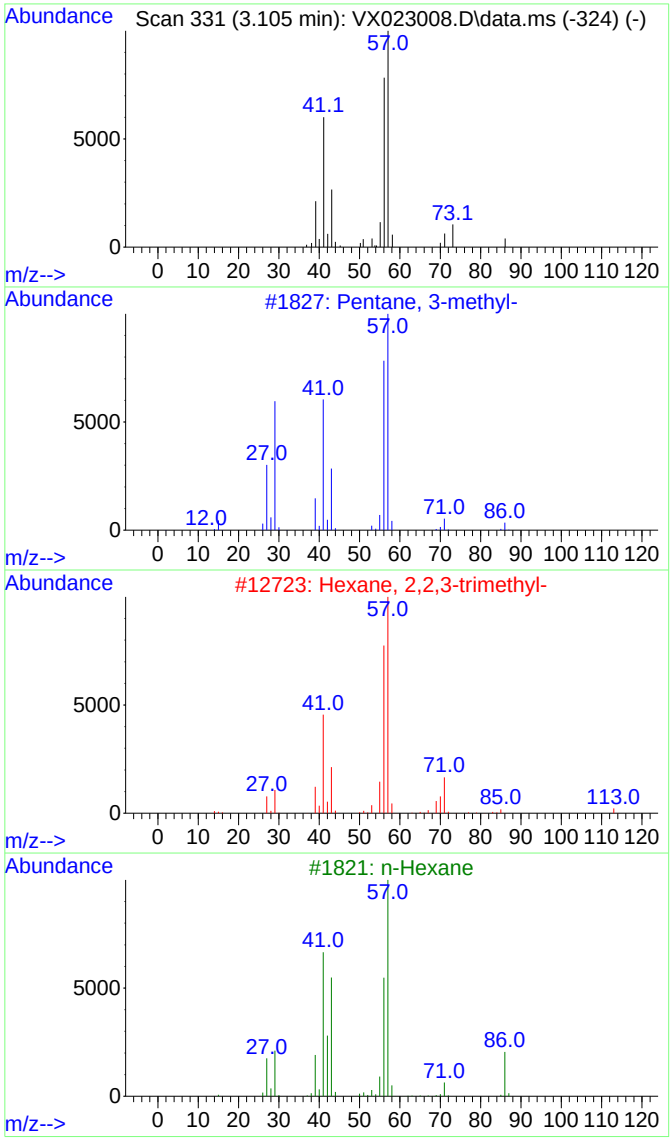
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

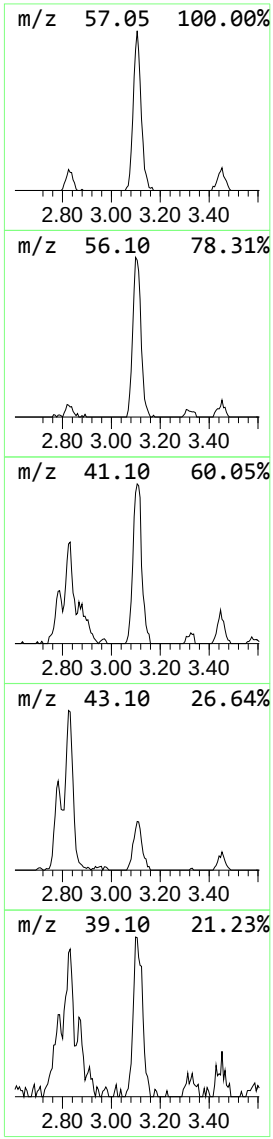
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.105	19.48 ug/l	67556	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56
3	n-Hexane	86	C6H14	000110-54-3	43
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

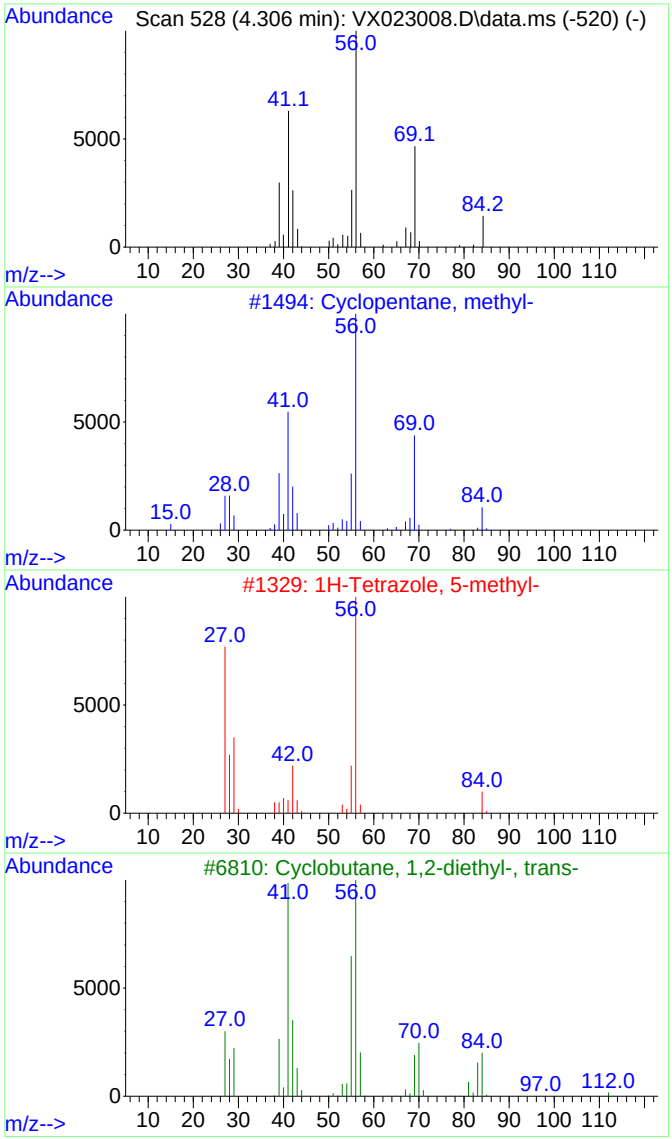
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

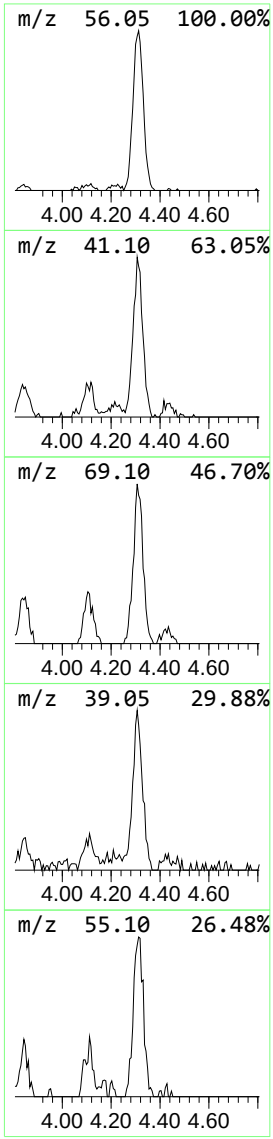
****

Peak Number 3 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	17.97 ug/l	62322	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	64
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

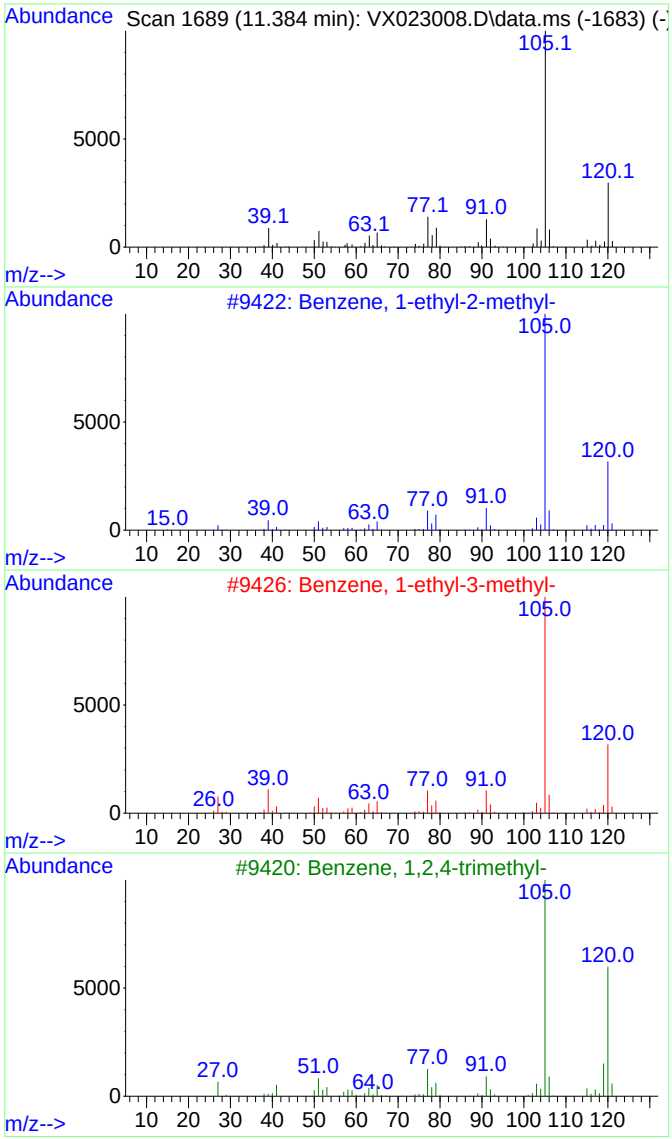
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

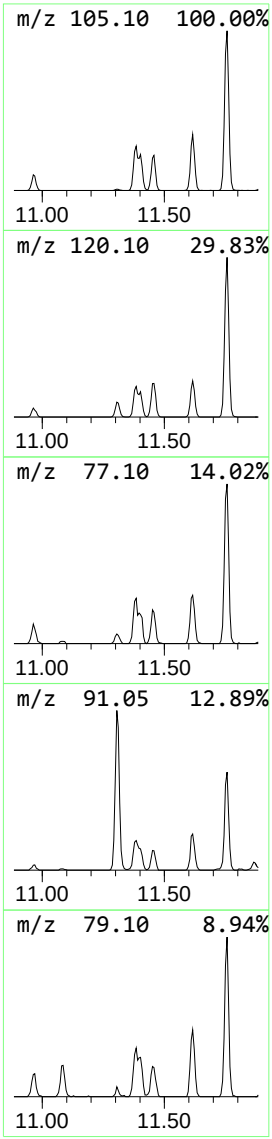
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	24.43 ug/l	141492	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-3-methyl-	120	C9H12	000620-14-4	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

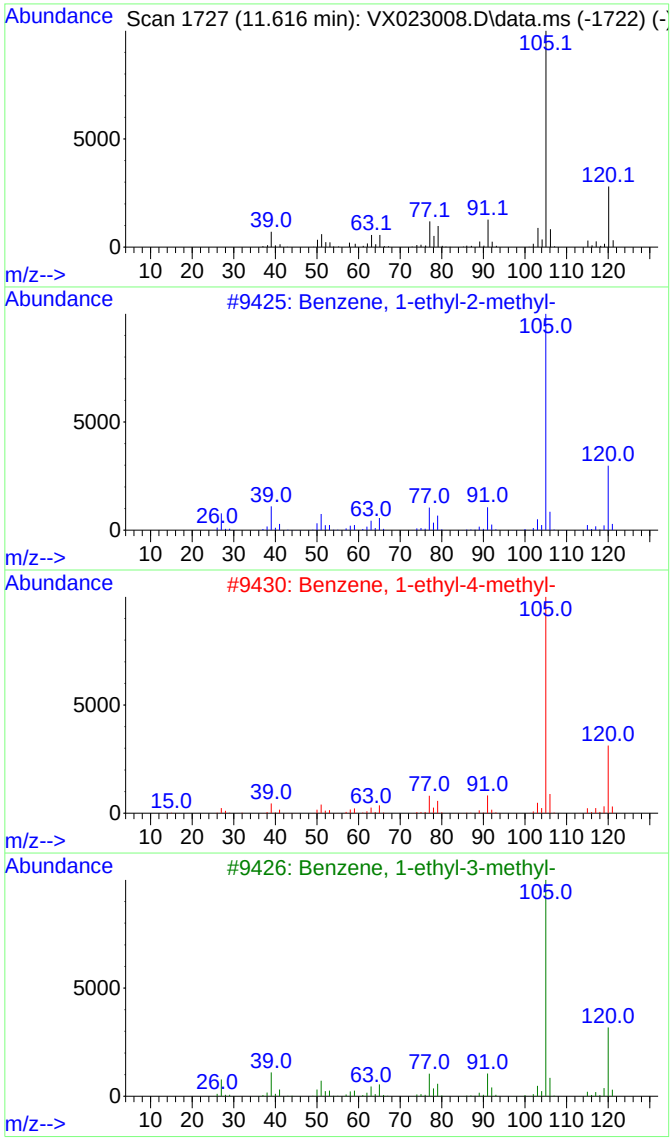
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

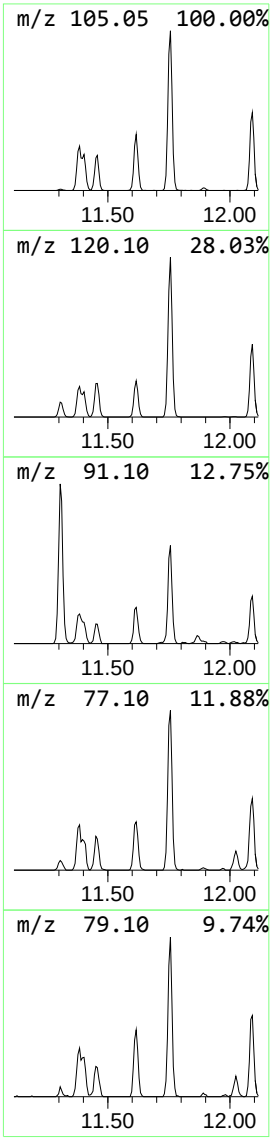
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	24.39 ug/l	141241	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	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

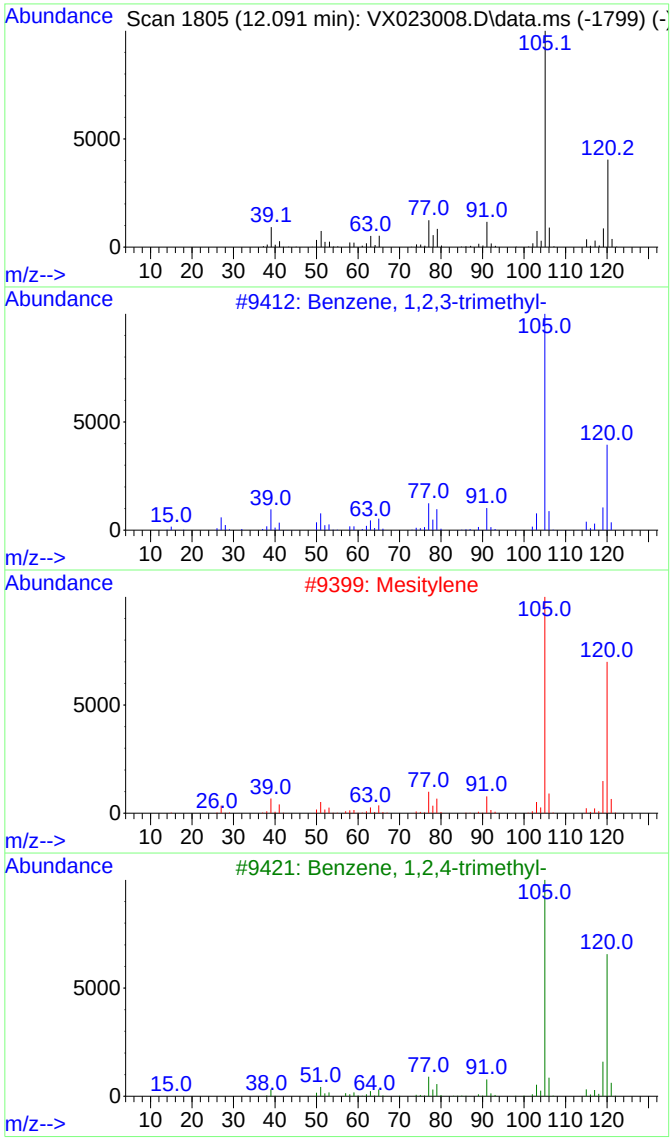
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

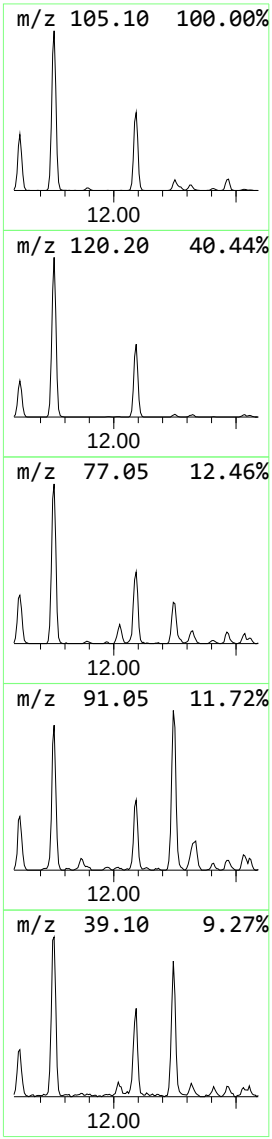
****

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	38.07 ug/l	220444	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

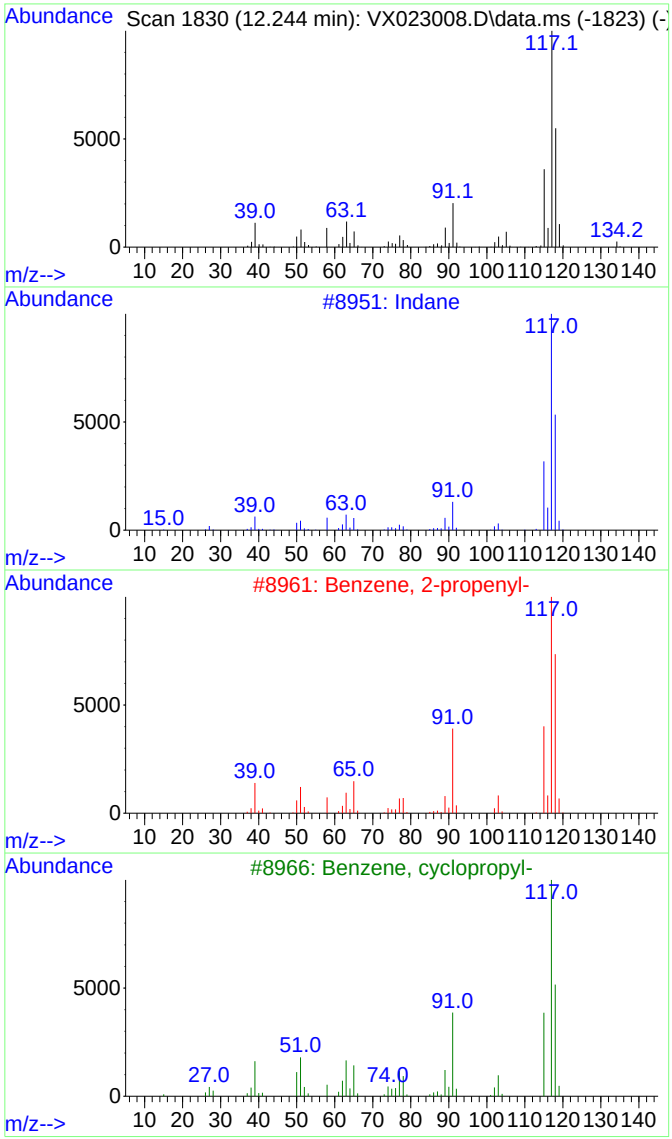
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

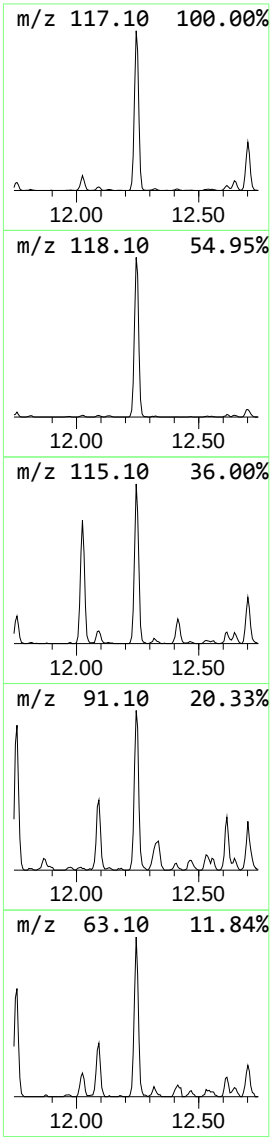
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	66.26 ug/l	383719	1,4-Dichlorobenzene-d4	12.024

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	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	74
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	62





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

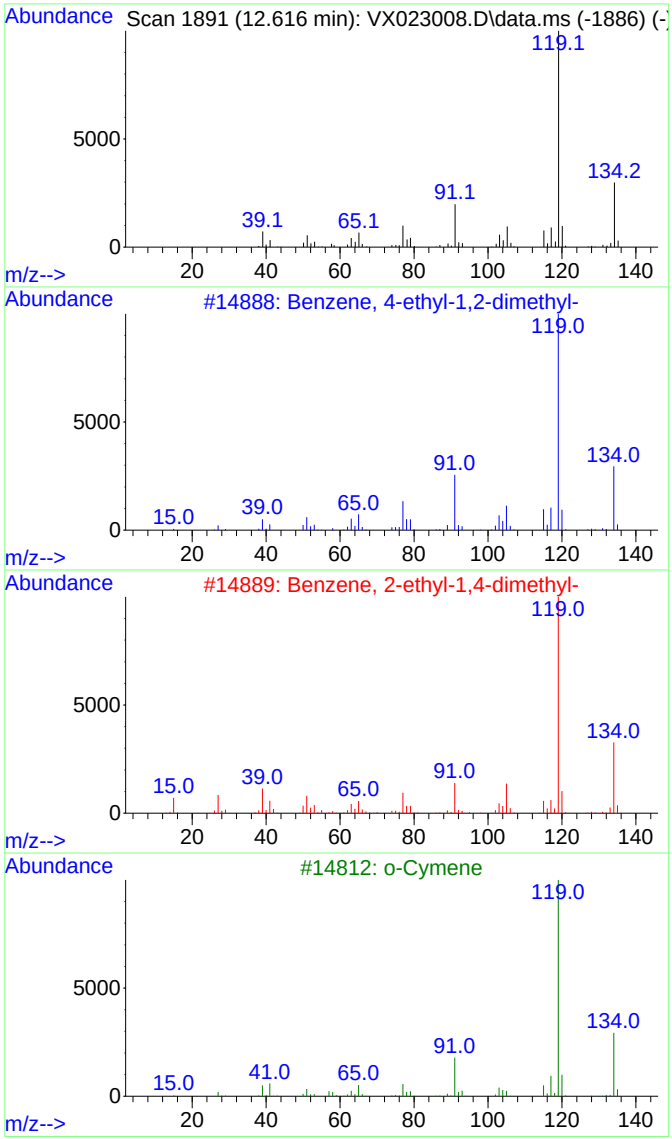
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

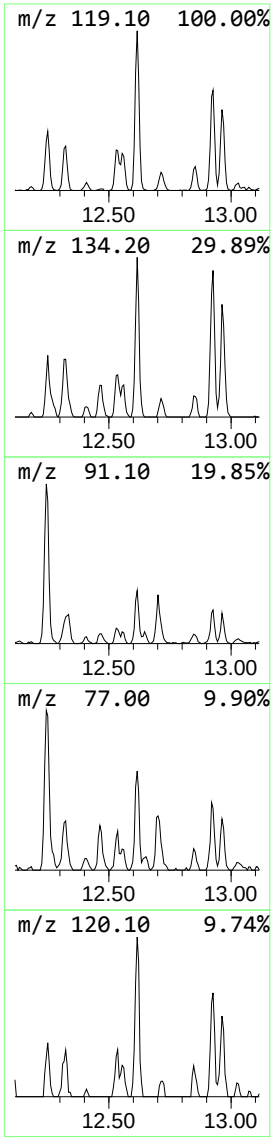
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	16.35 ug/l	94703	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3	o-Cymene	134	C10H14	000527-84-4	95
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
5	p-Cymene	134	C10H14	000099-87-6	95





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

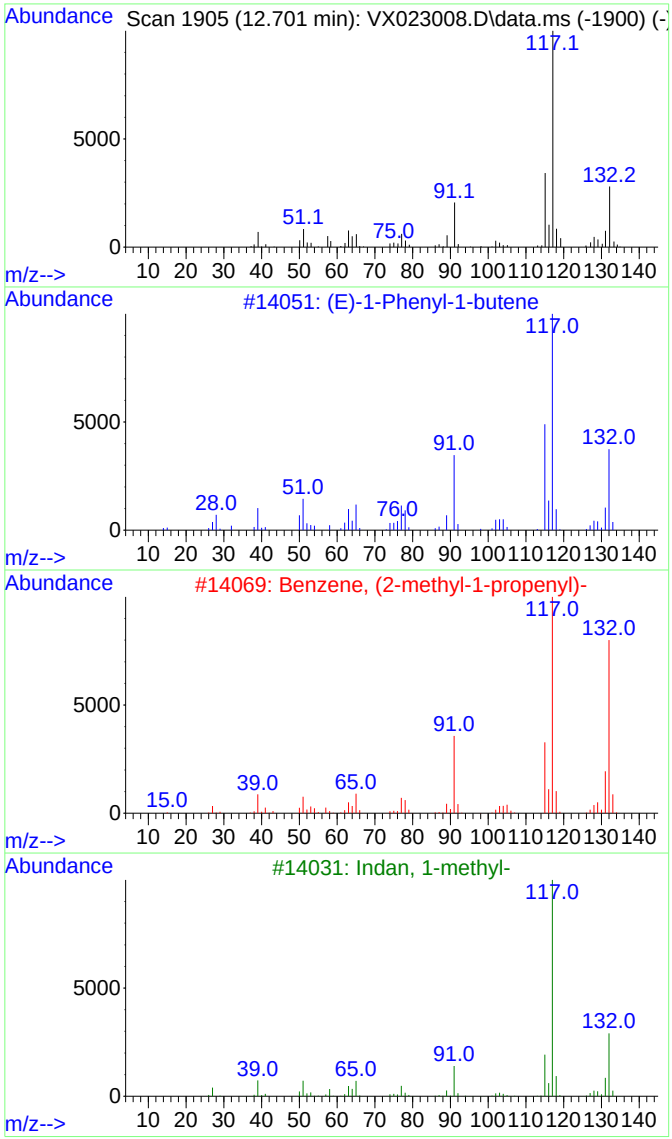
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

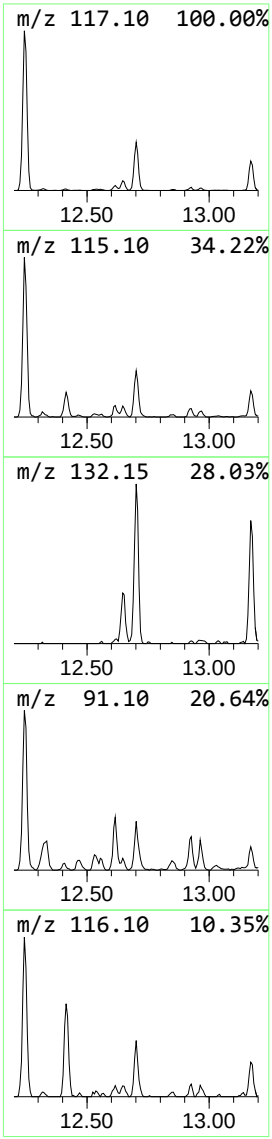
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (E)-1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	19.05 ug/l	110314	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	90
2	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	90
3	Indan, 1-methyl-	132	C10H12	000767-58-8	87
4	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-2

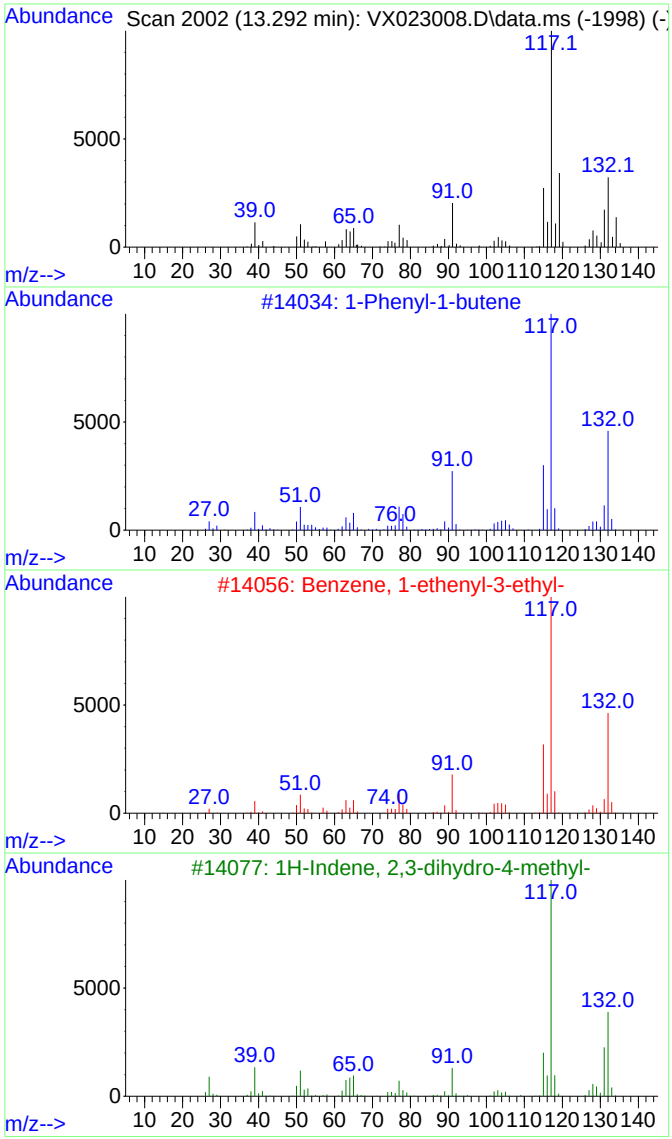
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

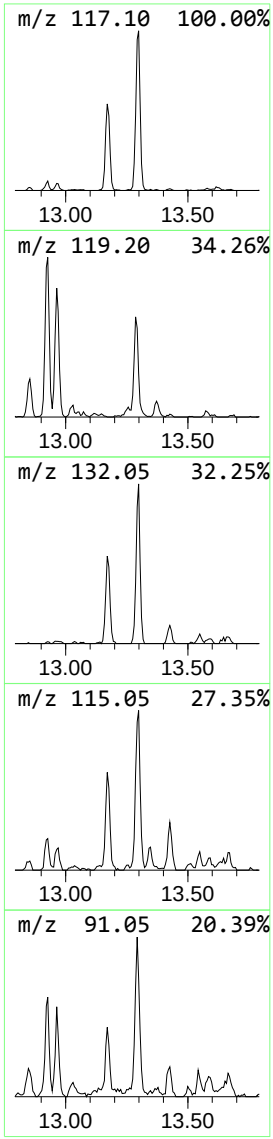
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	25.63 ug/l	148426	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	96
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	93
3	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062921\
Data File : VX023008.D
Acq On : 29 Jun 2021 17:06
Operator : JC/MD
Sample : M2875-17 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pentane, 2-methyl-	2.825	13.3	ug/l	46219	1	5.562	173393	50.0
Pentane, 3-methyl-	3.105	19.5	ug/l	67556	1	5.562	173393	50.0
Cyclopentane, m...	4.306	18.0	ug/l	62322	1	5.562	173393	50.0
Benzene, 1-ethy...	11.384	24.4	ug/l	141492	4	12.024	289556	50.0
Benzene, 1-ethy...	11.616	24.4	ug/l	141241	4	12.024	289556	50.0
Benzene, 1,2,3-...	12.091	38.1	ug/l	220444	4	12.024	289556	50.0
Indane	12.244	66.3	ug/l	383719	4	12.024	289556	50.0
Benzene, 4-ethy...	12.616	16.4	ug/l	94703	4	12.024	289556	50.0
(E)-1-Phenyl-1-...	12.701	19.1	ug/l	110314	4	12.024	289556	50.0
1-Phenyl-1-butene	13.292	25.6	ug/l	148426	4	12.024	289556	50.0