LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

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\82X043024W.M
Title : SW846 8260

Signal : TIC: VX041495.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	41	44	53	rVB2	5760	7305	1.03%	0.115%
2	1.569	69	79	81	rBV4	7104	19175	2.71%	0.301%
3	2.392	207	214	235	rBV	69195	145996	20.64%	2.290%
4	3.032	308	319	330	rVB3	3247	13313	1.88%	0.209%
5	4.227	504	515	523	rBV3	4098	13517	1.91%	0.212%
6	4.580	566	573	591	rBV	7614	27036	3.82%	0.424%
7	5.385	693	705	721	rBV2	79127	235582	33.30%	3.695%
8	5.550	721	732	749	rVB	140567	398050	56.26%	6.243%
9	5.952	785	798	815	rBV	87867	234210	33.10%	3.673%
10	6.647	901	912	922	rBV	20562	62079	8.77%	0.974%
11	6.757	922	930	949	rVB	213504	519485	73.42%	8.147%
12	6.964	956	964	981	rBV	132450	363079	51.32%	5.694%
13	7.470	1042	1047	1062	rVB	16071	41757	5.90%	0.655%
14	7.854	1102	1110	1113	rBV3	6933	14384	2.03%	0.226%
15	7.909	1114	1119	1130	rVB	13021	30291	4.28%	0.475%
16	8.586	1224	1230	1234	rBV	8761	16080	2.27%	0.252%
17	8.647	1234	1240	1251	rVB	455383	707506	100.00%	11.096%
18	8.811	1262	1267	1278	rVB2	10006	18617	2.63%	0.292%
19	8.945	1284	1289	1296	rBV	32942	55431	7.83%	0.869%
20	9.019	1296	1301	1311	rVB4	4629	11149	1.58%	0.175%
21	9.244	1332	1338	1349	rBV	23261	39329	5.56%	0.617%
22	9.451	1365	1372	1384	rBV	11036	21118	2.98%	0.331%
23	9.665	1401	1407	1409	rBV4	4096	7118	1.01%	0.112%
24	9.707	1409	1414	1424	rVB	30783	51942	7.34%	0.815%
25	9.799	1424	1429	1431	rBV2	5794	8673	1.23%	0.136%
26	9.835	1431	1435	1447	rVB	58857	85924	12.14%	1.348%
27	9.951	1449	1454	1461	rVB	9636	17277	2.44%	0.271%
28	10.055	1461	1471	1485	rBV	451225	634450	89.67%	9.951%
29	10.220	1489	1498	1503	rBV	20728	39604	5.60%	0.621%
30	10.274	1503	1507	1514	rVB	46571	65669	9.28%	1.030%
31	10.378	1520	1524	1533	rVB3	4016	8082	1.14%	0.127%
32	10.482	1536	1541	1546	rVV2	6707	10377	1.47%	0.163%
33	10.549	1548	1552	1564	rVB2	7351	14065	1.99%	0.221%
34	10.872	1599	1605	1611	rBV5	10365	26429	3.74%	0.415%
35	11.012	1623	1628	1630	rBV	14895	19977	2.82%	0.313%
36	11.079	1635	1639	1651	rVV	401884	579290	81.88%	9.085%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

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\82X043024W.M
Title : SW846 8260

37	11.177	1651	1655	1661	rVB2	12001	18865	2.67%	0.296%
38	11.293	1668	1674	1678	rBV2	12885	21316	3.01%	0.334%
39	11.341	1678	1682	1690	rVB4	11162	17993	2.54%	0.282%
40	11.414	1690	1694	1697	rBV3	7669	12033	1.70%	0.189%
41	11.457	1698	1701	1709	rVV3	6778	11919	1.68%	0.187%
42	11.530	1709	1713	1724	rVB2	11809	20714	2.93%	0.325%
43	11.713	1736	1743	1746	rBV	17727	24342	3.44%	0.382%
44	11.750	1746	1749	1754	rVB	9185	12536	1.77%	0.197%
45	11.908	1771	1775	1777	rBV	7890	9689	1.37%	0.152%
46	11.939	1777	1780	1782	rVV	13222	17140	2.42%	0.269%
47	11.969	1782	1785	1789	rVV	71080	92936	13.14%	1.458%
48	12.018	1789	1793	1806	rVV	487282	658875	93.13%	10.334%
49	12.140	1808	1813	1817	rVB5	5470	10206	1.44%	0.160%
50	12.353	1841	1848	1856	rBV4	15293	40576	5.74%	0.636%
51	12.518	1870	1875	1883	rVB	12724	20351	2.88%	0.319%
52	12.701	1901	1905	1914	rVB	22568	31783	4.49%	0.498%
53	12.835	1920	1927	1932	rVB8	4289	10050	1.42%	0.158%
54	13.006	1950	1955	1959	rBV4	6371	12093	1.71%	0.190%
55	13.054	1959	1963	1970	rVV	13094	20587	2.91%	0.323%
56	13.378	2012	2016	2021	rBV2	17944	26929	3.81%	0.422%
57	13.554	2039	2045	2048	rBV4	6493	13628	1.93%	0.214%
58	13.591	2048	2051	2062	rVB4	4062	11077	1.57%	0.174%
59	13.810	2083	2087	2093	rVB3	9050	12360	1.75%	0.194%
60	14.097	2129	2134	2140	rBV	94119	128976	18.23%	2.023%
61	14.152	2140	2143	2149	rVB5	7621	13984	1.98%	0.219%
62	14.493	2195	2199	2204	rBV3	6481	11933	1.69%	0.187%
63	14.688	2226	2231	2237	rBV5	10417	21362	3.02%	0.335%
64	14.847	2253	2257	2267	rVB2	10781	19597	2.77%	0.307%
65	15.011	2280	2284	2290	rBV	26159	44522	6.29%	0.698%
66	15.176	2308	2311	2315	rVB3	8720	11032	1.56%	0.173%
67	15.237	2315	2321	2326	rBV	15825	24652	3.48%	0.387%
68	15.456	2353	2357	2360	rBV	10028	14433	2.04%	0.226%
69	15.487	2360	2362	2367	rVB	14124	18304	2.59%	0.287%
70	15.725	2394	2401	2406	rVB2	14446	27579	3.90%	0.433%
71	15.822	2412	2417	2420	rBV2	13145	23244	3.29%	0.365%
72	15.932	2430	2435	2438	rBV2	5479	8225	1.16%	0.129%
73	16.011	2442	2448	2452	rBV	53090	103516	14.63%	1.624%
74	16.212	2475	2481	2488	rBV	21438	45431	6.42%	0.713%
75	16.286	2488	2493	2499	rVV2	15263	26743	3.78%	0.419%
76	16.359	2500	2505	2515	rVB	23049	44808	6.33%	0.703%

LSC Area Percent Report

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Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Title : SW846 8260

77	16.596	2538	2544	2548	rBV2	20024	36989	5.23%	0.580%
78	16.645	2548	2552	2562	rVB	17838	37821	5.35%	0.593%
79	16.743	2562	2568	2573	rBV2	9098	21518	3.04%	0.337%

Sum of corrected areas: 6376033

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
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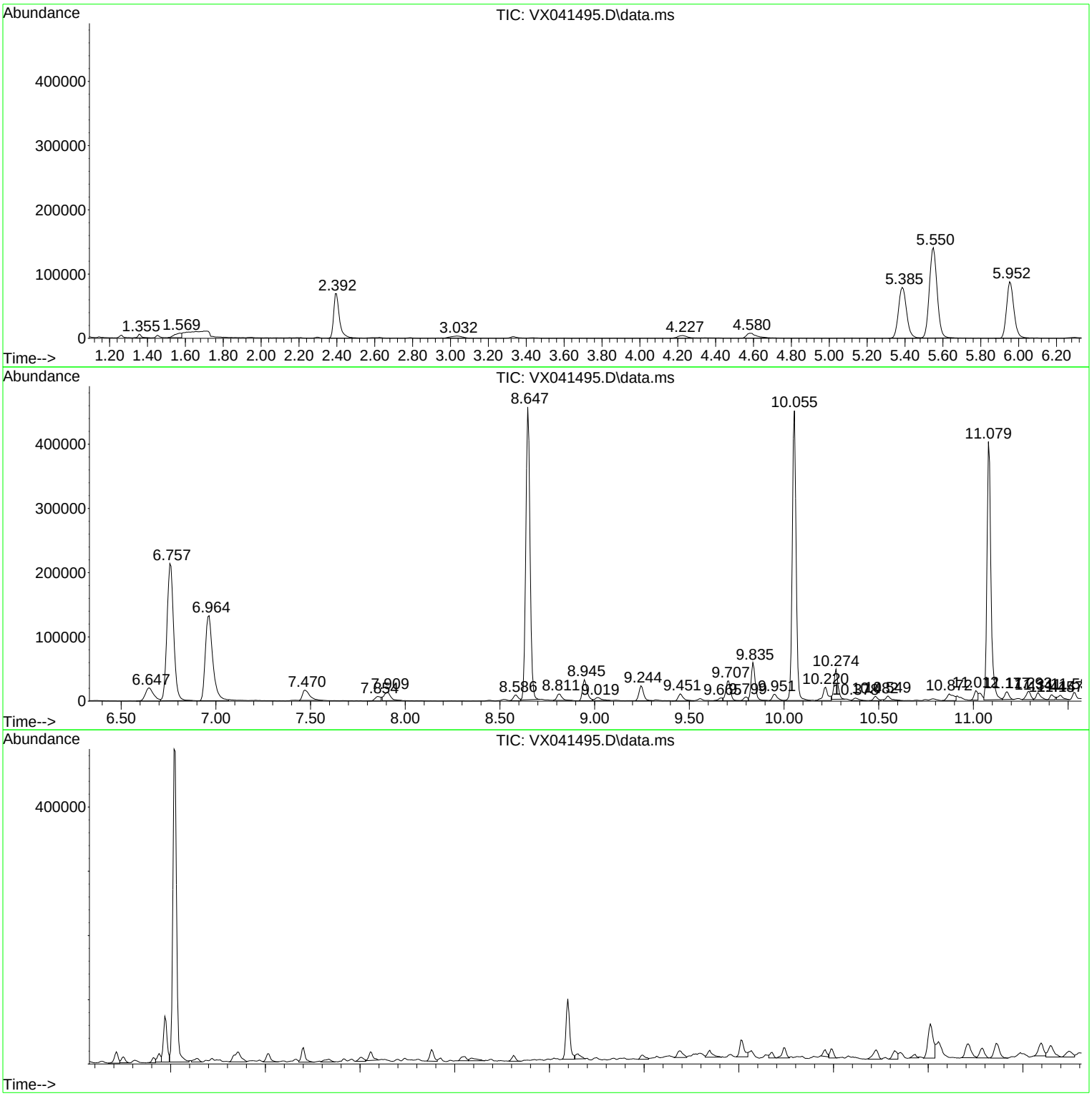
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

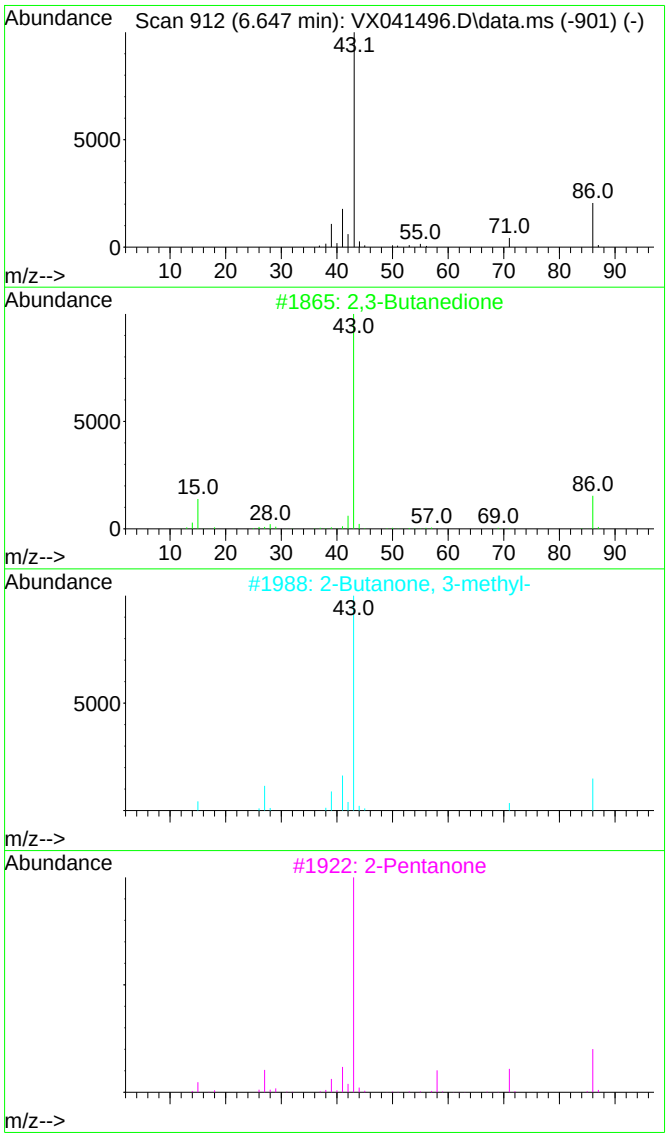
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

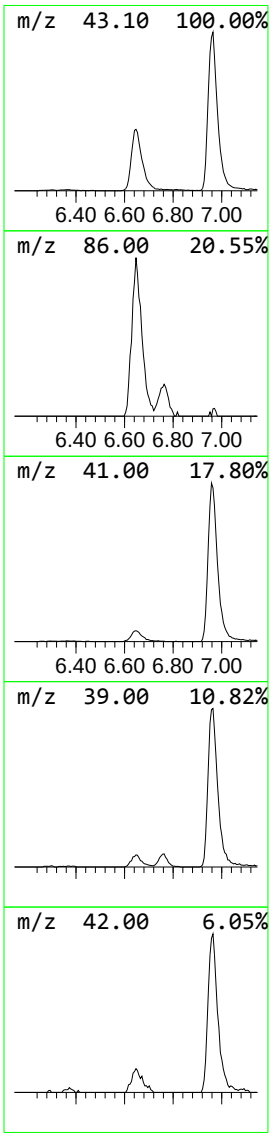
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,3-Butanedione Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.647	5.98 ug/l	62079	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	80
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
3	2-Pentanone	86	C5H10O	000107-87-9	64
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	38
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

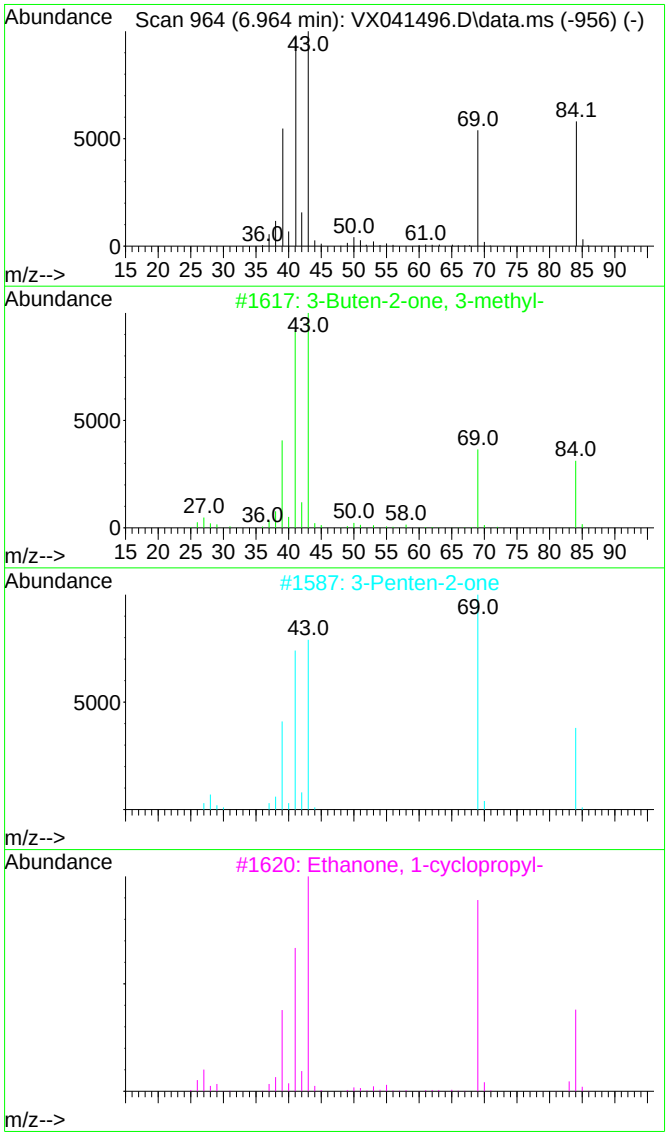
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

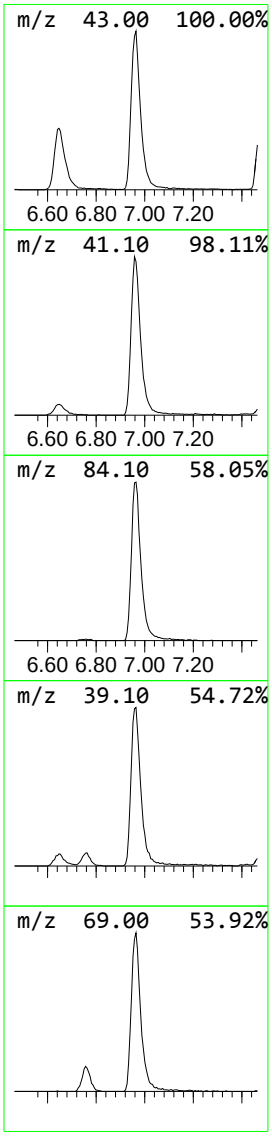
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Buten-2-one, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.964	34.95 ug/l	363079	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	3-Penten-2-one	84	C5H8O	000625-33-2	90
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	58
4	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	43
5	Methacrolein	70	C4H6O	000078-85-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

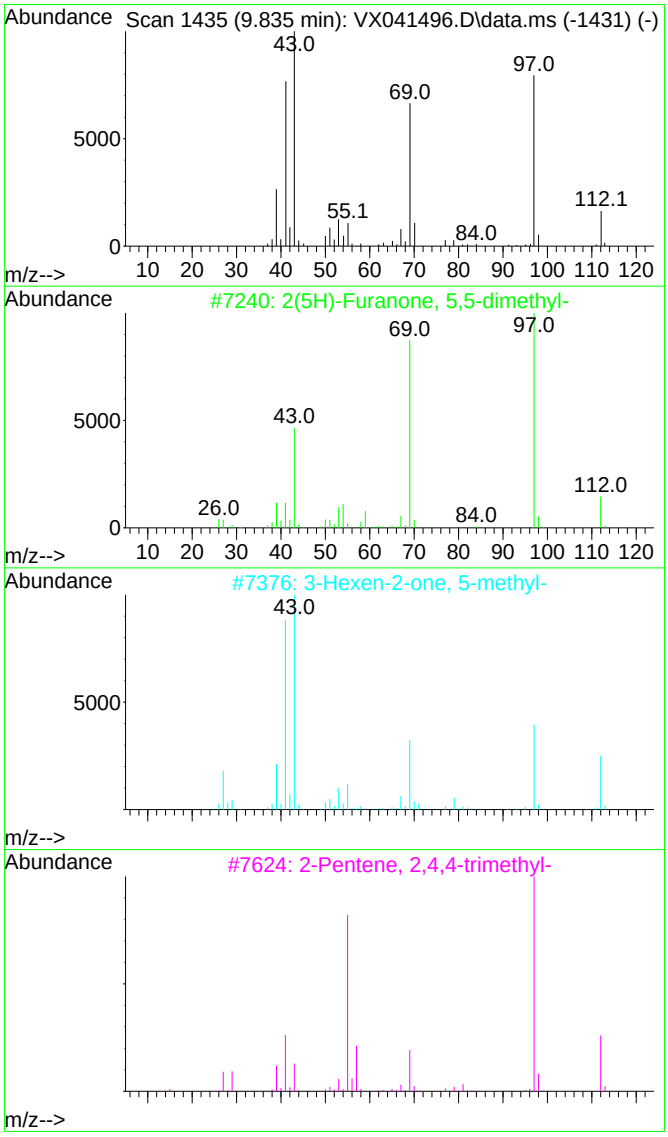
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

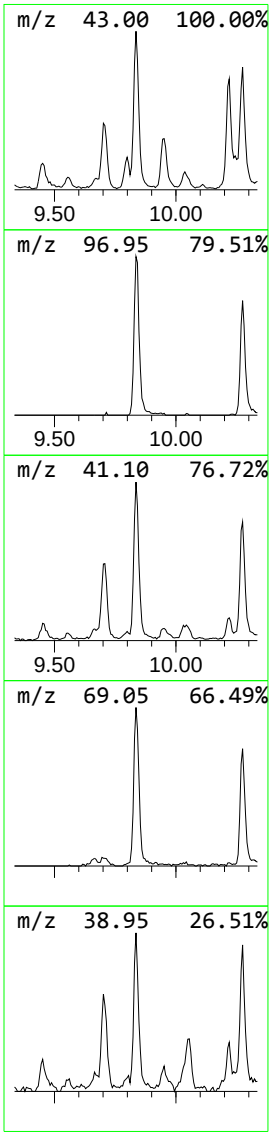
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2(5H)-Furanone, 5,5-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.835	6.77 ug/l	85924	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	74
2	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	53
3	2-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-40-4	50
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	50
5	Cyclopentanecarboxylic acid, 4-n...	235	C12H13NO4	1000307-58-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

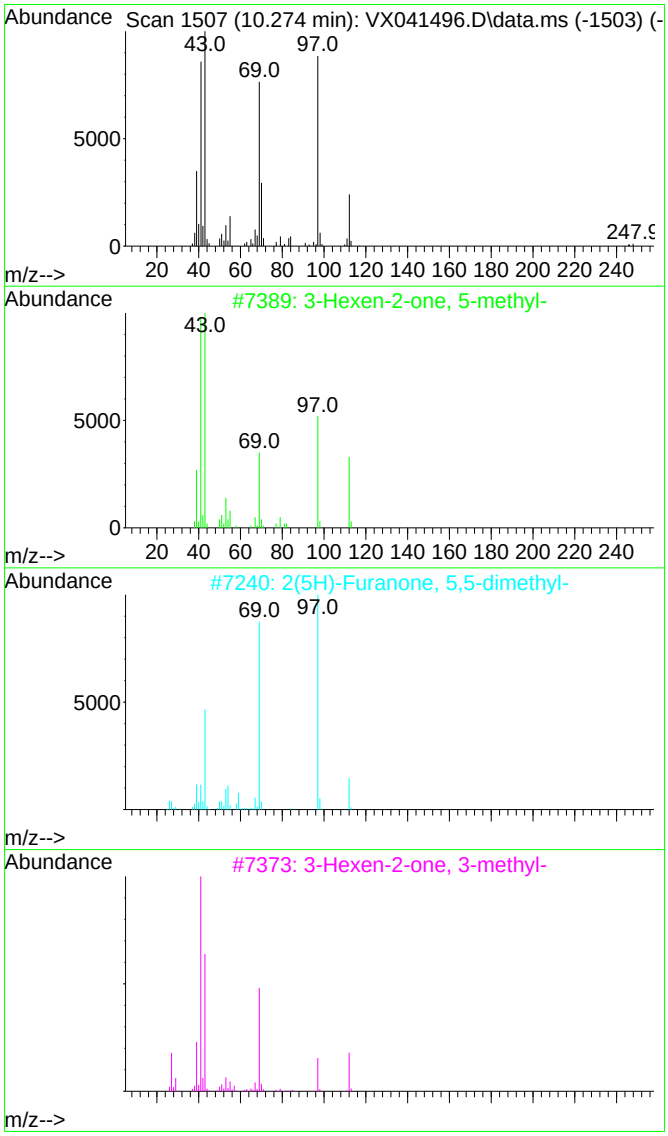
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

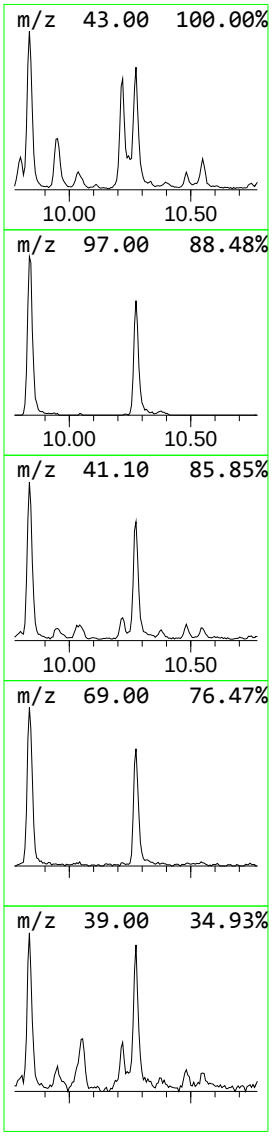
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Hexen-2-one, 5-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.274	5.18 ug/l	65669	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	72
2	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	72
3	3-Hexen-2-one, 3-methyl-	112	C7H12O	001187-80-0	46
4	2-Methyl-2-heptene	112	C8H16	000627-97-4	46
5	2-Pentene, 3,4,4-trimethyl-	112	C8H16	000598-96-9	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

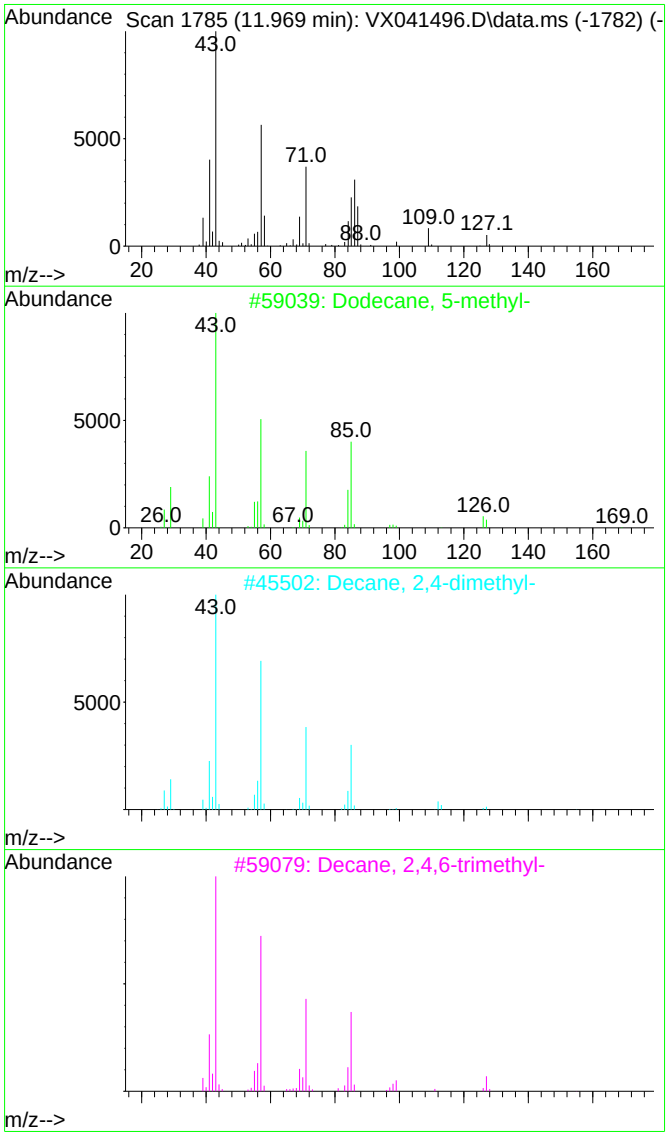
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

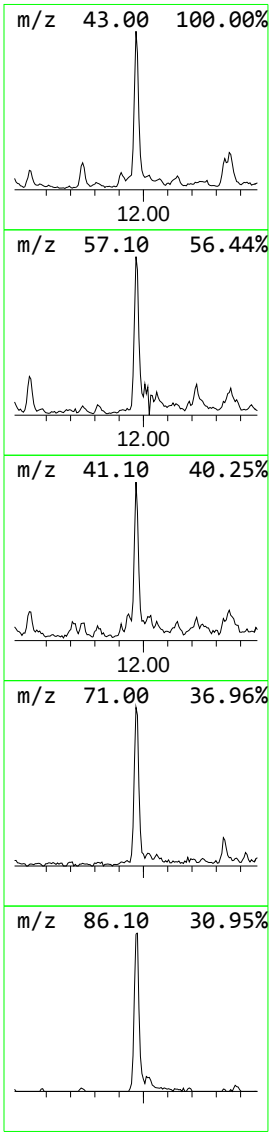
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown11.969 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	7.05 ug/l	92936	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 5-methyl-	184	C13H28	017453-93-9	43
2	Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	43
3	Decane, 2,4,6-trimethyl-	184	C13H28	062108-27-4	40
4	Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	38
5	Carbonic acid, nonyl prop-1-en-2...	228	C13H24O3	1000382-53-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

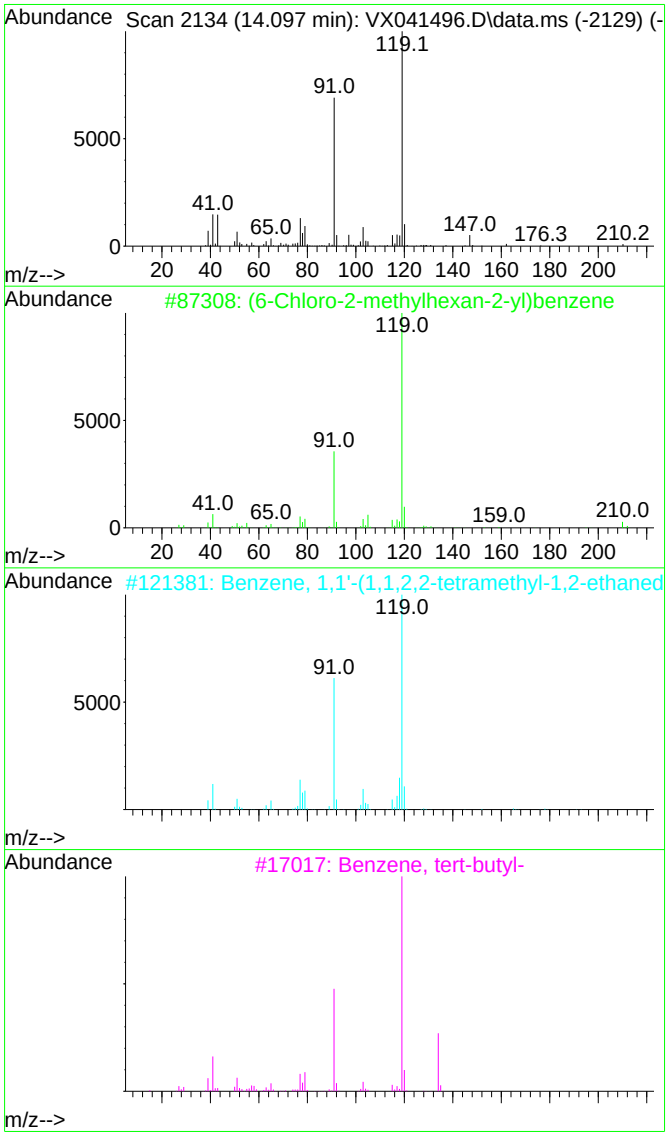
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

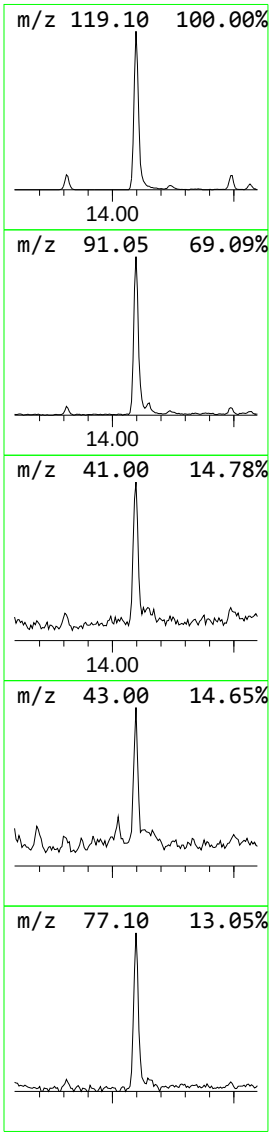
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (6-Chloro-2-methylhexan-2-y... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.097	9.79 ug/l	128976	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	90
2	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	87
3	Benzene, tert-butyl-	134	C10H14	000098-06-6	78
4	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	78
5	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

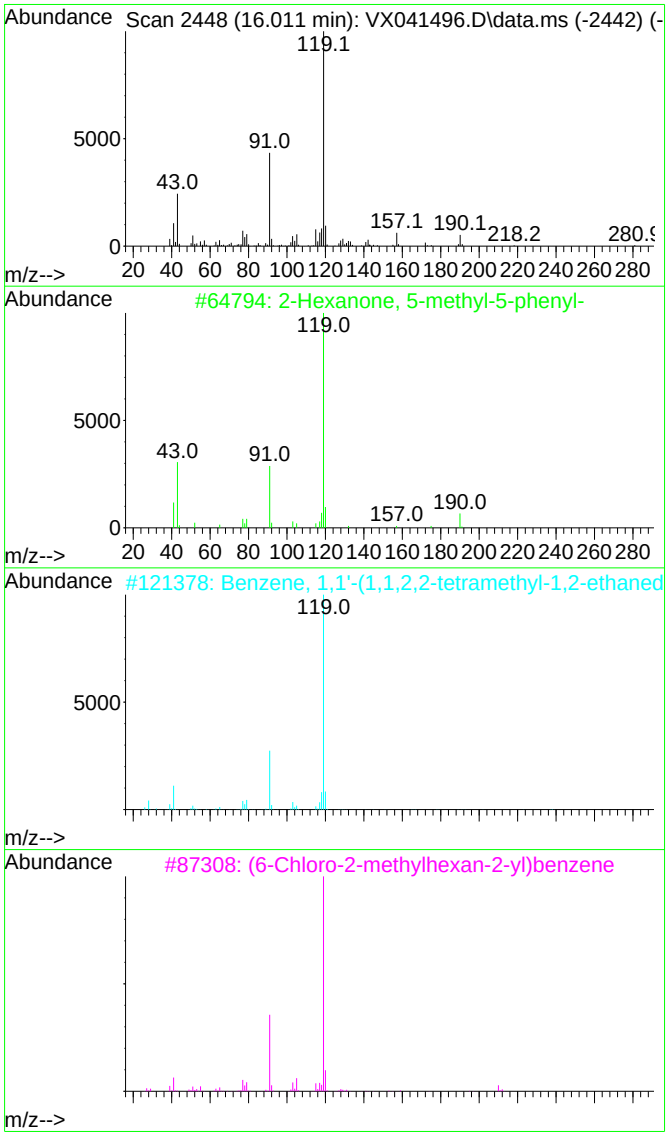
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.M
Quant Title : SW846 8260

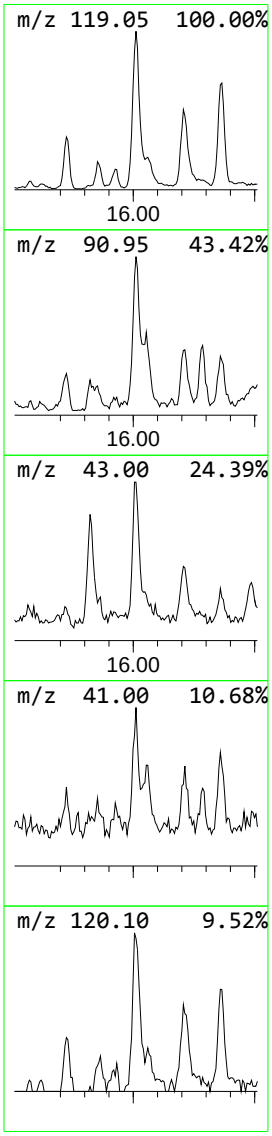
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Hexanone, 5-methyl-5-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.011	7.86 ug/l	103516	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 5-methyl-5-phenyl-	190	C13H18O	014128-61-1	80
2	Benzene, 1,1'-(1,1,2,2-tetrameth...	238	C18H22	001889-67-4	72
3	(6-Chloro-2-methylhexan-2-yl)ben...	210	C13H19Cl	1417621-45-4	72
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	72
5	1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051324\
Data File : VX041496.D
Acq On : 13 May 2024 16:36
Operator : JC/MD
Sample : P2454-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SP25-06-20240510-WC

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X043024W.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
2,3-Butanedione	6.647	6.0	ug/l	62079	2	6.757	519485	50.0
3-Buten-2-one, ...	6.964	35.0	ug/l	363079	2	6.757	519485	50.0
2(5H)-Furanone,...	9.835	6.8	ug/l	85924	3	10.055	634450	50.0
3-Hexen-2-one, ...	10.274	5.2	ug/l	65669	3	10.055	634450	50.0
unknown11.969	11.969	7.0	ug/l	92936	4	12.024	658875	50.0
(6-Chloro-2-met...	14.097	9.8	ug/l	128976	4	12.024	658875	50.0
2-Hexanone, 5-m...	16.011	7.9	ug/l	103516	4	12.024	658875	50.0