

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052225\
 Data File : VX046316.D
 Acq On : 22 May 2025 10:03
 Operator : JC/MD
 Sample : Q2102-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 LAW-25-0078

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\82X050525W.M
 Title : SW846 8260

Signal : TIC: VX046316.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	51	rVB2	5536	6658	1.57%	0.193%
2	1.605	79	85	88	rVB5	5581	11673	2.75%	0.339%
3	2.386	207	213	224	rVB	9257	18290	4.31%	0.531%
4	2.965	298	308	321	rBV3	6375	17210	4.06%	0.500%
5	5.385	694	705	719	rBV	49835	148526	35.01%	4.311%
6	5.544	721	731	747	rVV2	70592	202467	47.72%	5.877%
7	5.952	787	798	814	rBV	58869	157337	37.08%	4.567%
8	6.757	922	930	944	rBV	124912	305922	72.10%	8.880%
9	6.958	955	963	969	rBV6	3689	8539	2.01%	0.248%
10	7.903	1112	1118	1124	rBV2	2350	4809	1.13%	0.140%
11	8.513	1212	1218	1223	rBV4	3170	5245	1.24%	0.152%
12	8.647	1232	1240	1250	rBV	269611	424289	100.00%	12.316%
13	9.171	1321	1326	1333	rBV2	4119	7655	1.80%	0.222%
14	9.244	1333	1338	1341	rBV2	3957	6425	1.51%	0.187%
15	9.378	1356	1360	1365	rBV2	3796	5847	1.38%	0.170%
16	9.445	1365	1371	1384	rVV	30828	49175	11.59%	1.427%
17	9.586	1384	1394	1403	rVV2	28830	46607	10.98%	1.353%
18	10.049	1465	1470	1483	rVB	271459	391661	92.31%	11.369%
19	10.146	1483	1486	1492	rVB7	2726	4325	1.02%	0.126%
20	10.372	1518	1523	1532	rVB	139359	187297	44.14%	5.437%
21	10.549	1547	1552	1556	rBV2	7906	11625	2.74%	0.337%
22	10.860	1598	1603	1607	rBV	22223	32206	7.59%	0.935%
23	10.896	1607	1609	1613	rVB2	3768	4496	1.06%	0.131%
24	11.012	1622	1628	1632	rVB4	6064	11258	2.65%	0.327%
25	11.079	1632	1639	1648	rBV	232461	302302	71.25%	8.775%
26	11.152	1648	1651	1655	rVB3	5308	6992	1.65%	0.203%
27	11.335	1678	1681	1685	rBV2	4218	5347	1.26%	0.155%
28	11.451	1696	1700	1704	rBV	10841	14493	3.42%	0.421%
29	11.530	1708	1713	1719	rVB	32186	44938	10.59%	1.304%
30	11.695	1736	1740	1744	rBV5	8470	13713	3.23%	0.398%
31	11.738	1744	1747	1754	rVB4	4502	8965	2.11%	0.260%
32	11.890	1768	1772	1774	rBV5	3214	4941	1.16%	0.143%
33	11.939	1776	1780	1783	rVV2	9333	13695	3.23%	0.398%
34	11.975	1783	1786	1789	rVV2	16030	25355	5.98%	0.736%
35	12.018	1789	1793	1805	rVV	278024	348231	82.07%	10.109%
36	12.201	1818	1823	1832	rBV7	4495	12173	2.87%	0.353%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.347	1839	1847	1851	rBV4	10972	24217	5.71%	0.703%
38	12.439	1856	1862	1865	rBV8	2273	5599	1.32%	0.163%
39	12.597	1882	1888	1891	rVB7	3114	5494	1.29%	0.159%
40	12.658	1891	1898	1908	rBV	55264	98080	23.12%	2.847%
41	12.750	1911	1913	1917	rVB4	4314	5073	1.20%	0.147%
42	12.835	1922	1927	1932	rBV2	14998	22104	5.21%	0.642%
43	12.951	1942	1946	1949	rBV2	7755	9361	2.21%	0.272%
44	12.994	1949	1953	1959	rVB	16009	20542	4.84%	0.596%
45	13.061	1959	1964	1970	rVV7	3797	8330	1.96%	0.242%
46	13.134	1970	1976	1982	rVB6	3886	7811	1.84%	0.227%
47	13.268	1994	1998	2002	rBV2	26179	33138	7.81%	0.962%
48	13.371	2011	2015	2018	rBV3	4238	5660	1.33%	0.164%
49	13.585	2043	2050	2053	rBV8	2645	5596	1.32%	0.162%
50	13.628	2053	2057	2060	rVV5	4006	7122	1.68%	0.207%
51	13.664	2060	2063	2071	rVB	9089	14353	3.38%	0.417%
52	13.780	2078	2082	2086	rBV2	2605	5514	1.30%	0.160%
53	14.060	2121	2128	2132	rVB9	3805	7894	1.86%	0.229%
54	14.140	2134	2141	2143	rBV7	2767	4640	1.09%	0.135%
55	14.432	2186	2189	2193	rBV6	3570	5522	1.30%	0.160%
56	14.493	2193	2199	2205	rVB9	4761	8944	2.11%	0.260%
57	14.609	2215	2218	2221	rBV4	5019	6968	1.64%	0.202%
58	15.207	2307	2316	2323	rBV	99630	158812	37.43%	4.610%
59	15.414	2348	2350	2354	rVB3	6888	7403	1.74%	0.215%
60	15.487	2358	2362	2366	rBV7	8670	17480	4.12%	0.507%
61	15.572	2372	2376	2380	rBV5	9876	18039	4.25%	0.524%
62	16.084	2455	2460	2468	rBV2	32377	60537	14.27%	1.757%

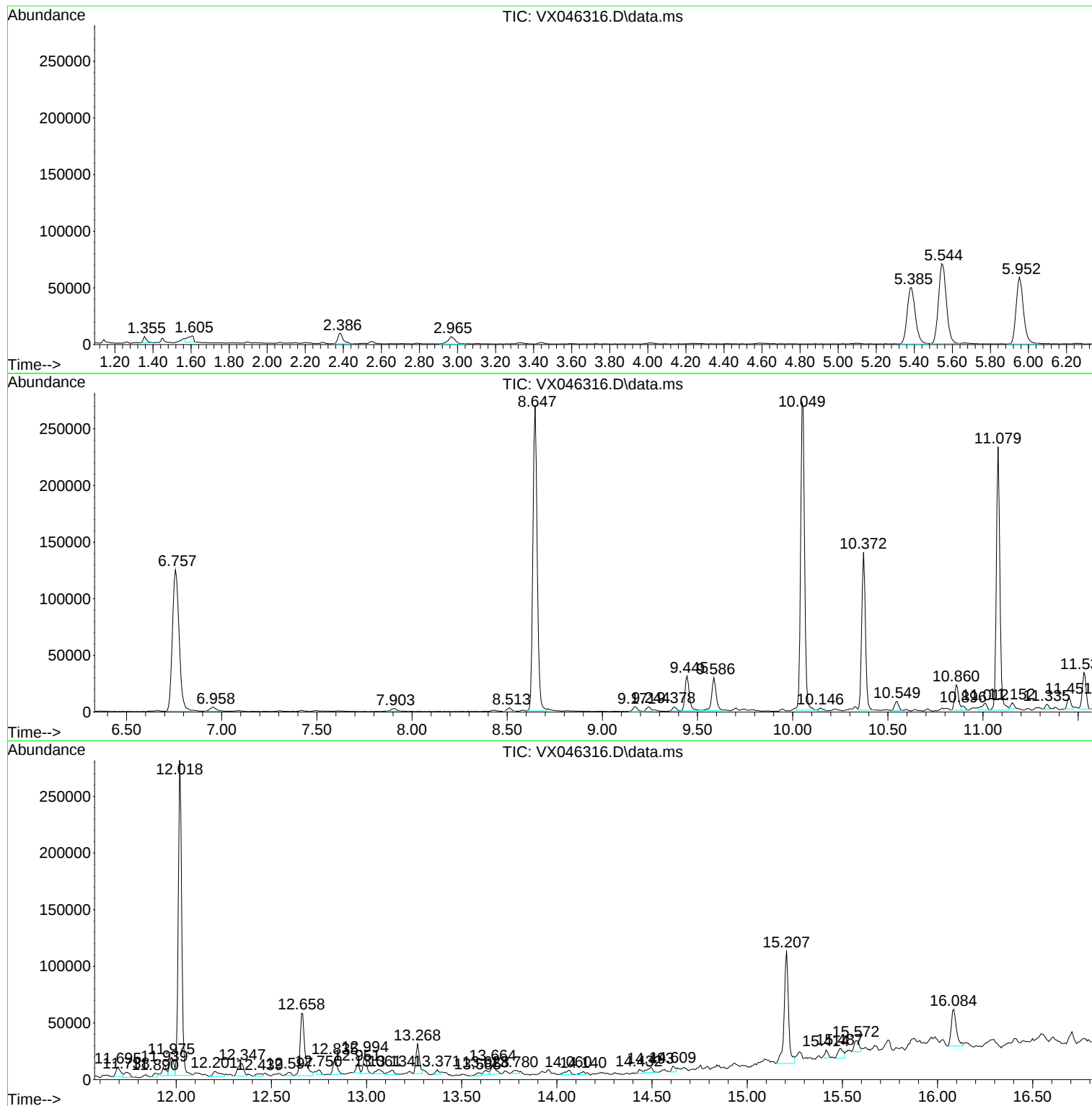
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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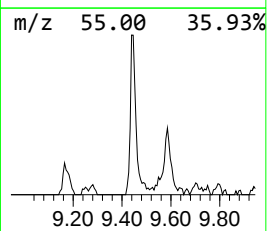
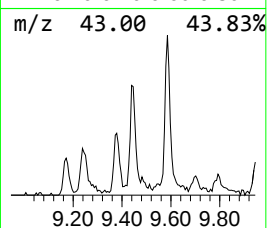
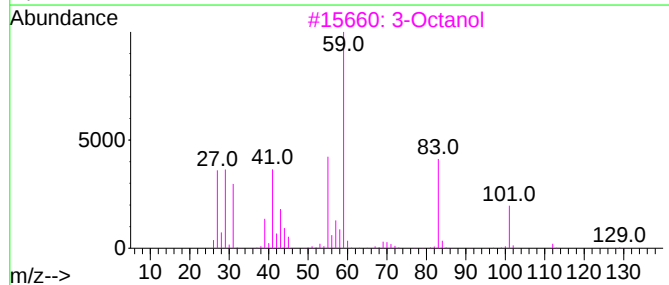
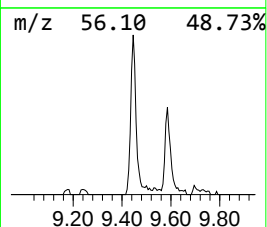
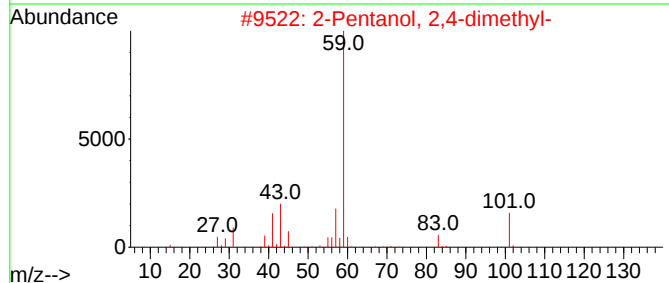
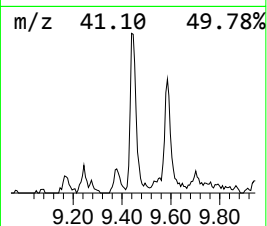
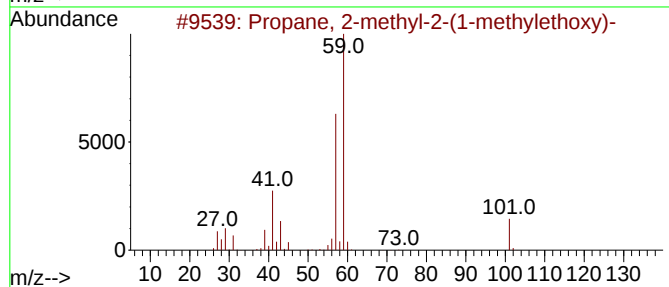
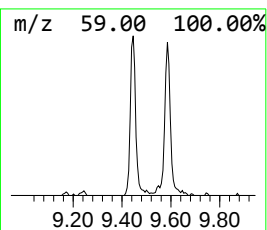
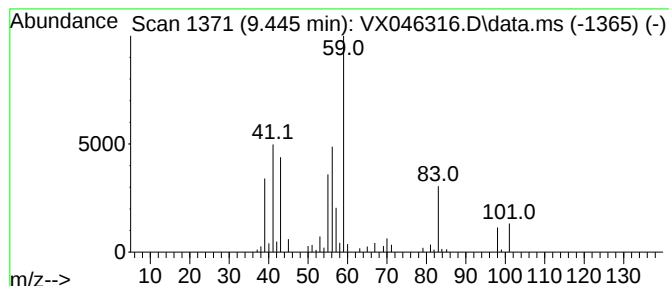
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown9.445 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.445	6.28 ug/l	49175	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	43
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38
3			3-Octanol	130	C8H18O	000589-98-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	28



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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LAW-25-0078

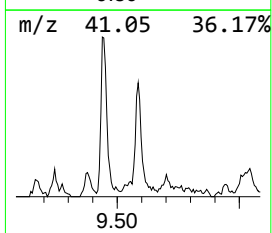
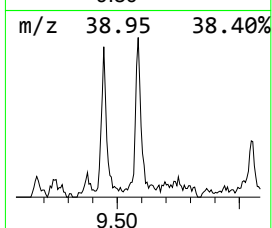
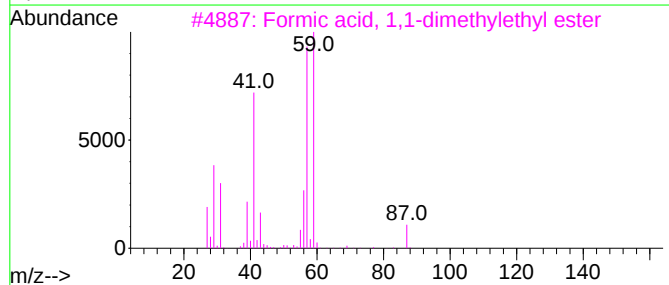
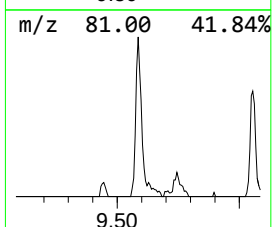
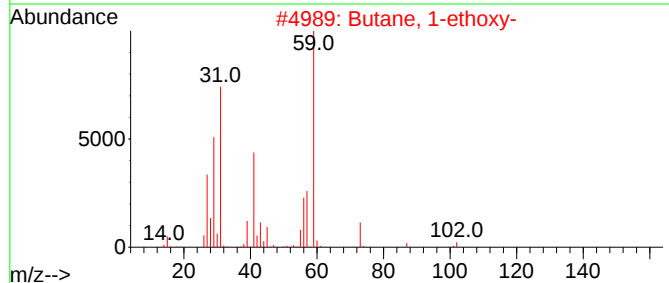
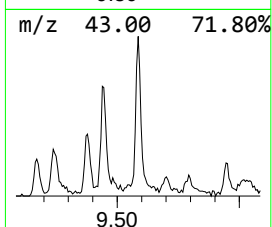
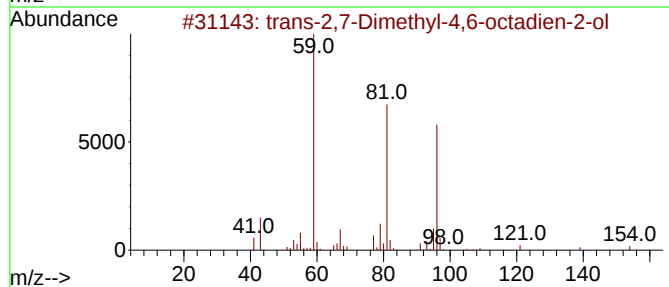
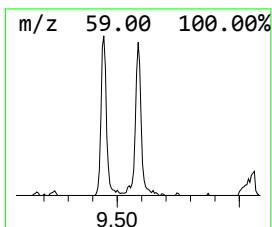
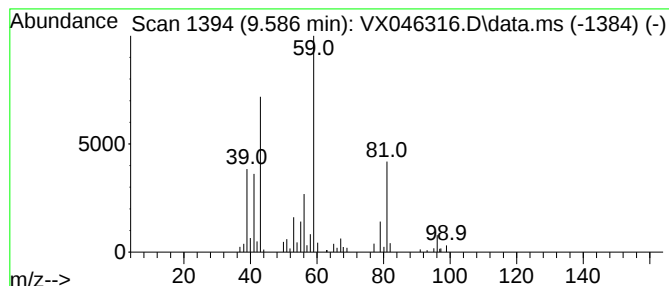
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 2 trans-2,7-Dimethyl-4,6-octa... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.586	5.95 ug/l	46607	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	53
2			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	37
3			Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	25
4			o-Menthan-8-ol	156	C10H20O	343855-44-7	23
5			2-Hydroxy-2,6-dimethyl-hept-6-en...	156	C9H16O2	001068-82-2	23



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ALS Vial : 7 Sample Multiplier: 1

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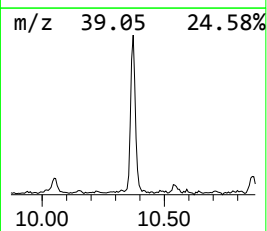
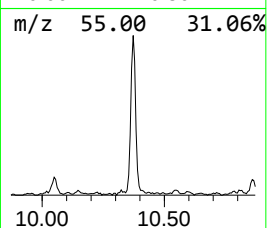
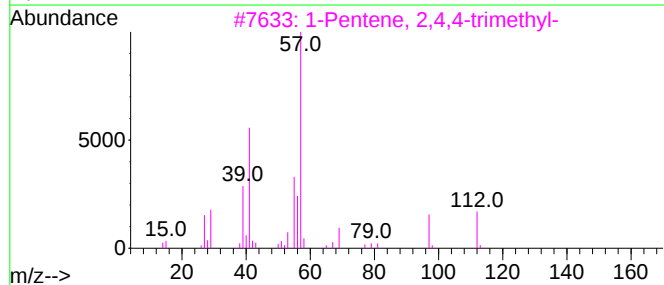
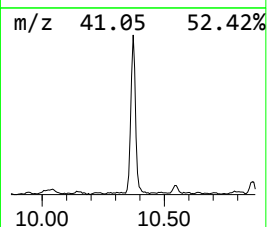
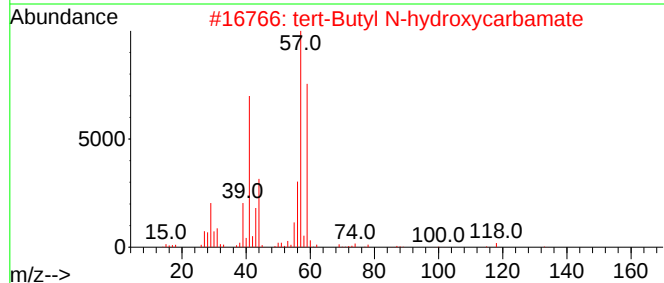
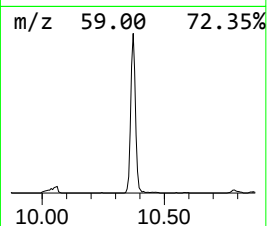
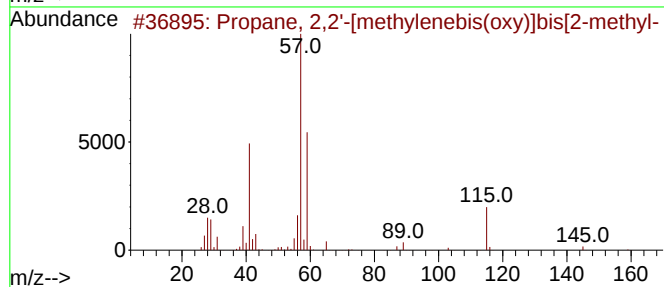
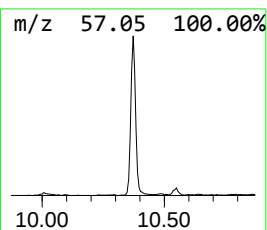
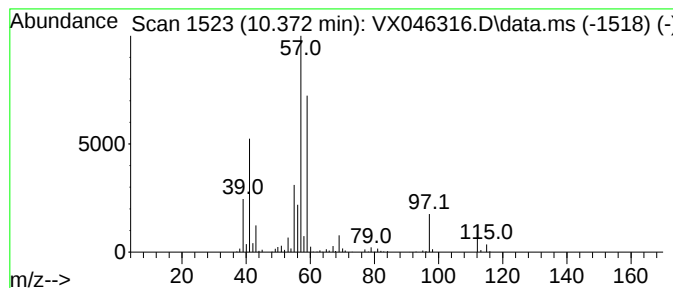
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Quant Title : SW846 8260

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

Peak Number 3 Propane, 2,2'-[methylenebis... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.372	23.91 ug/l	187297	Chlorobenzene-d5	10.049

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2'-[methylenebis(oxy)...	160	C9H20O2	002568-93-6	59
2			tert-Butyl N-hydroxycarbamate	133	C5H11NO3	036016-38-3	53
3			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	49
4			1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	43
5			Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	42



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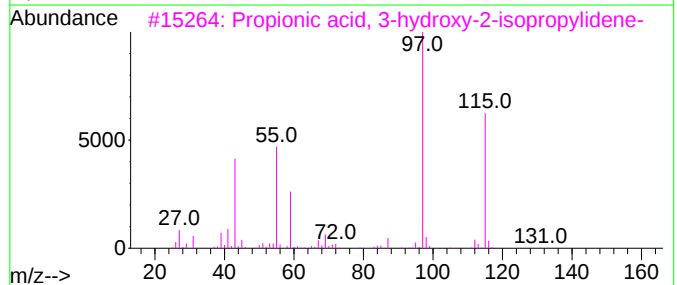
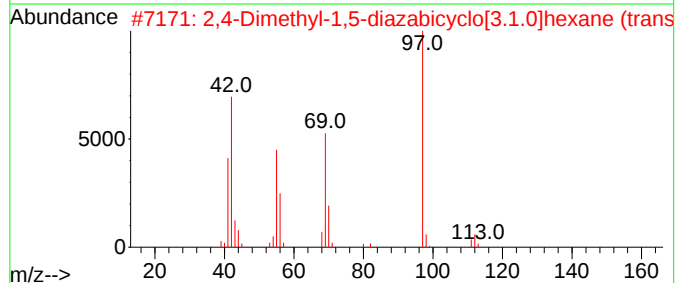
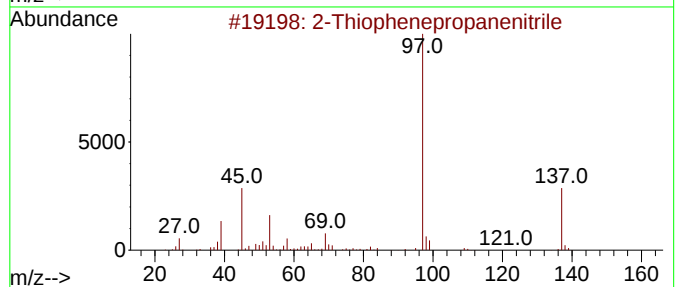
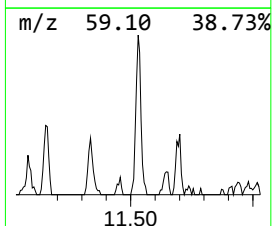
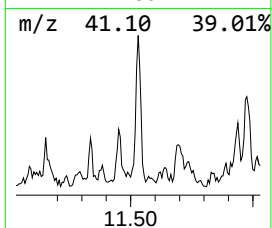
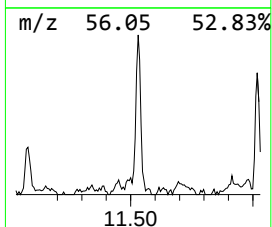
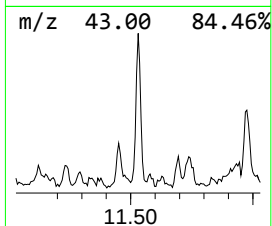
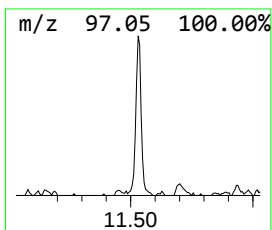
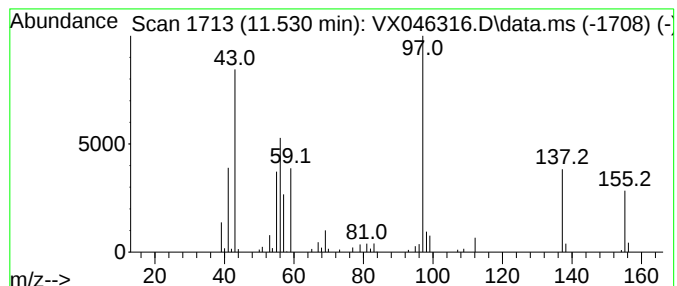
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 4 unknown11.530 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.530	6.45 ug/l	44938	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Thiophenepropanenitrile	137	C7H7NS	005722-13-4	38
2			2,4-Dimethyl-1,5-diazabicyclo[3.1.0]hexane (trans)	112	C6H12N2	1000283-20-9	35
3			Propionic acid, 3-hydroxy-2-isopropylidene-	130	C6H10O3	1000153-27-1	32
4			1H-Pyrazol-4-amine, 3-methyl-	97	C4H7N3	1010338-28-2	32
5			Cyclohexanone, 3-butyl-	154	C10H18O	039178-69-3	27



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ClientSampleId :
LAW-25-0078

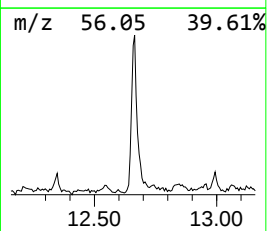
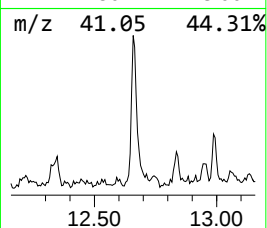
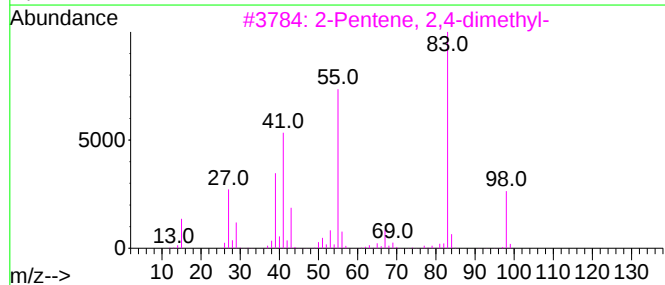
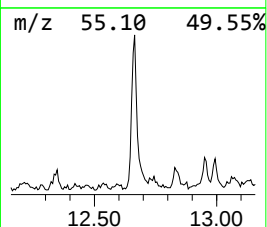
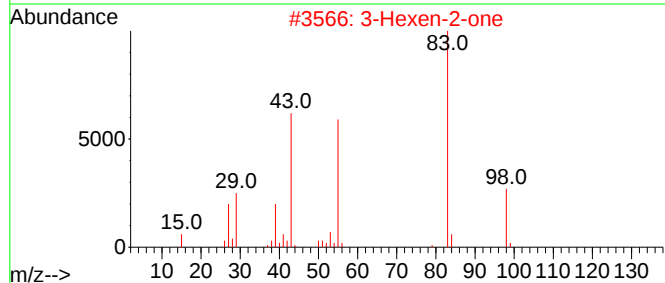
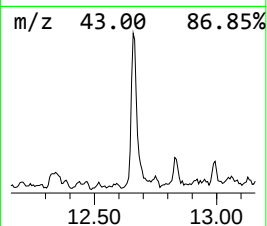
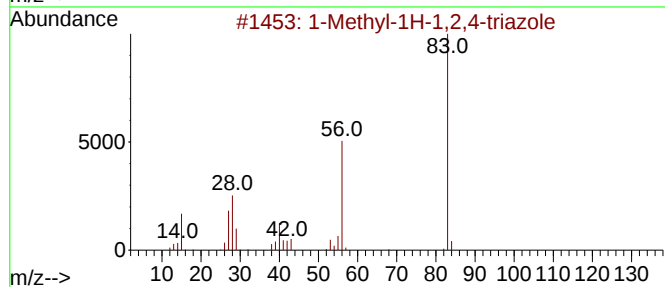
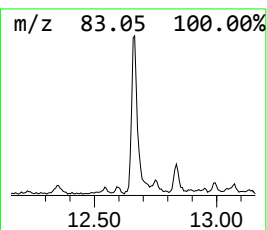
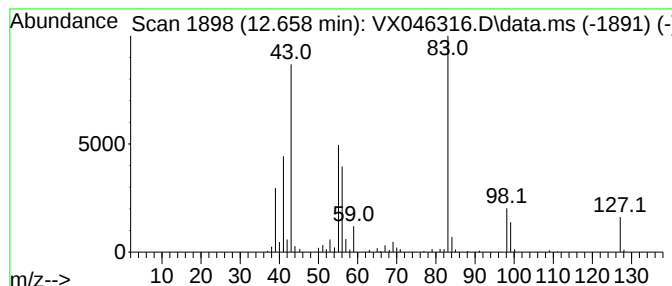
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Quant Title : SW846 8260

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

Peak Number 5 1-Methyl-1H-1,2,4-triazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.658	14.08 ug/l	98080	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	50
2			3-Hexen-2-one	98	C6H10O	000763-93-9	49
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	49
4			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	47
5			1-Butene, 2,3,3-trimethyl-	98	C7H14	000594-56-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052225\
Data File : VX046316.D
Acq On : 22 May 2025 10:03
Operator : JC/MD
Sample : Q2102-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LAW-25-0078

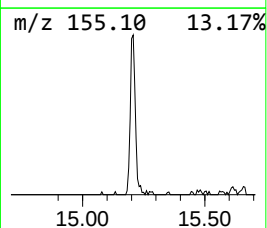
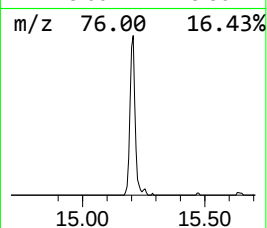
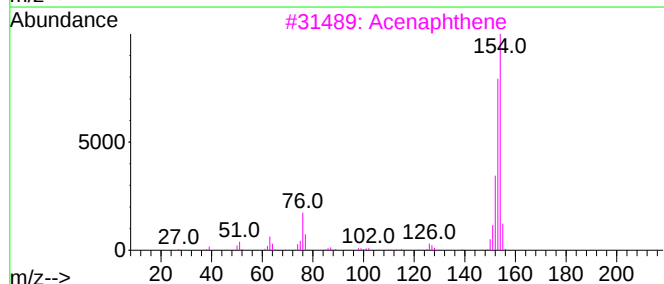
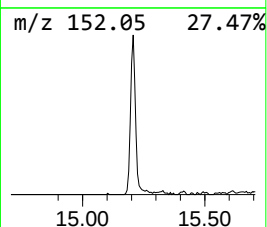
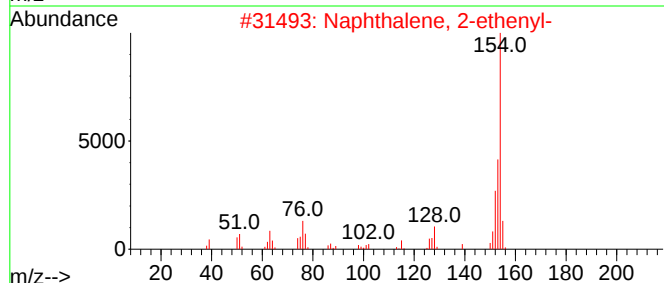
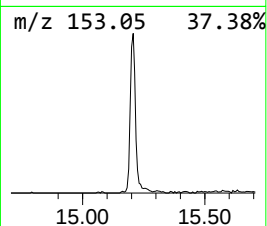
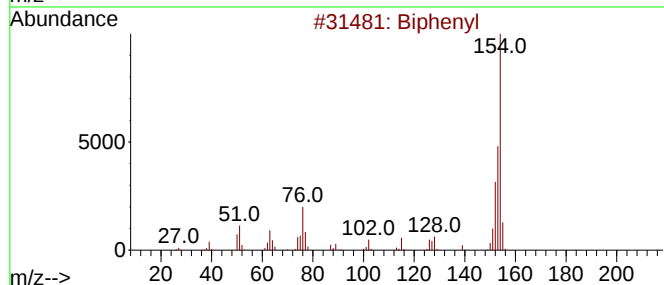
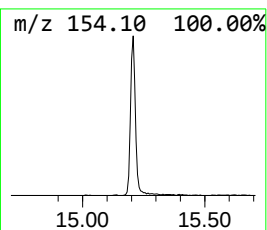
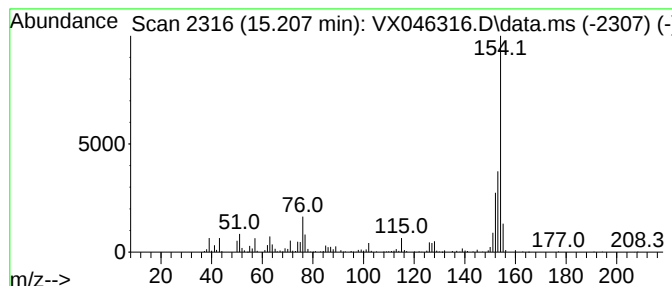
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Quant Title : SW846 8260

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

Peak Number 6 Biphenyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	22.80 ug/l	158812	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	96
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	74
3			Acenaphthene	154	C12H10	000083-32-9	64
4			3-Quinolincarbonitrile	154	C10H6N2	034846-64-5	53
5			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052225\
Data File : VX046316.D
Acq On : 22 May 2025 10:03
Operator : JC/MD
Sample : Q2102-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LAW-25-0078

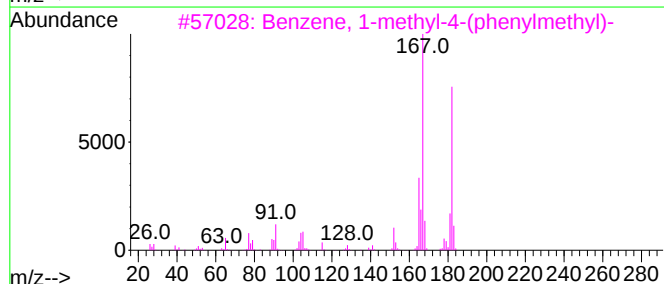
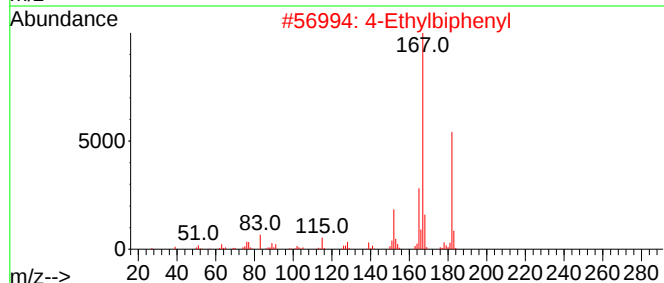
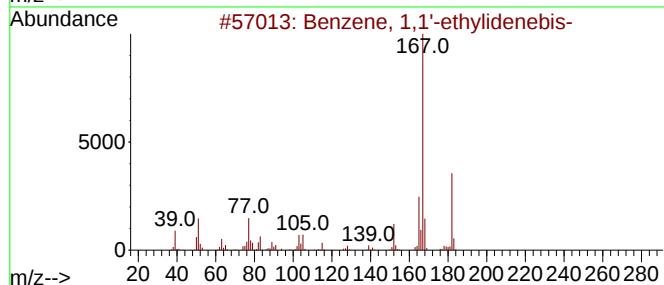
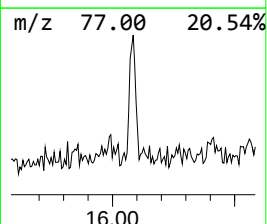
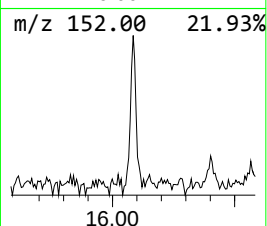
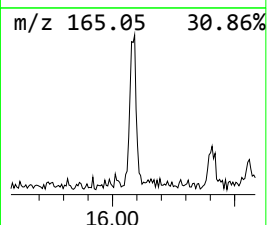
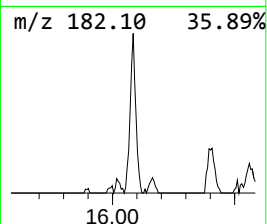
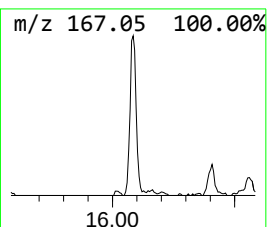
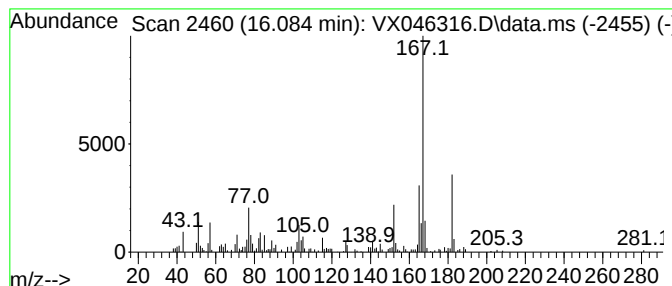
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1,1'-ethylidenebis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.084	8.69 ug/l	60537	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-ethylidenebis-	182	C14H14	000612-00-0	96
2			4-Ethylbiphenyl	182	C14H14	005707-44-8	81
3			Benzene, 1-methyl-4-(phenylmethyl)-	182	C14H14	000620-83-7	68
4			Benzene, 1-methyl-2-(phenylmethyl)-	182	C14H14	000713-36-0	64
5			Benzene, 1,1'-(chloromethylene)bis-	202	C13H11Cl	000090-99-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052225\
Data File : VX046316.D
Acq On : 22 May 2025 10:03
Operator : JC/MD
Sample : Q2102-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
LAW-25-0078

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X050525W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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trans-2,7-Dimet...	9.586	6.0	ug/l	46607	3	10.049	391661	50.0
Propane, 2,2'-[...	10.372	23.9	ug/l	187297	3	10.049	391661	50.0
unknown11.530	11.530	6.5	ug/l	44938	4	12.018	348231	50.0
1-Methyl-1H-1,2...	12.658	14.1	ug/l	98080	4	12.018	348231	50.0
Biphenyl	15.207	22.8	ug/l	158812	4	12.018	348231	50.0
Benzene, 1,1'-e...	16.084	8.7	ug/l	60537	4	12.018	348231	50.0