LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090623\
Data File : VX037554.D
Acq On : 06 Sep 2023 15:00
Operator : JC/MD
Sample : 04220-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

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\82X081723W.M
Title : SW846 8260

Signal : TIC: VX037554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	56	59	65	rBV	20421	23553	1.15%	0.215%
2	2.386	206	213	222	rBV2	14644	26180	1.28%	0.239%
3	2.965	296	308	322	rBV2	354782	909871	44.48%	8.290%
4	3.117	322	333	352	rVB	595546	1372192	67.08%	12.502%
5	3.763	431	439	453	rVB	43204	112873	5.52%	1.028%
6	4.300	512	527	541	rVB3	14337	48438	2.37%	0.441%
7	4.586	556	574	596	rBV	656704	2045503	100.00%	18.636%
8	5.007	633	643	665	rBV	215517	672345	32.87%	6.126%
9	5.391	694	706	714	rBV	72811	216358	10.58%	1.971%
10	5.470	715	719	724	rVV	12610	32375	1.58%	0.295%
11	5.550	724	732	753	rVB	135363	394145	19.27%	3.591%
12	5.958	790	799	806	rBV	77269	204912	10.02%	1.867%
13	6.037	806	812	823	rVV	87272	232843	11.38%	2.121%
14	6.172	823	834	838	rVV3	18799	62277	3.04%	0.567%
15	6.239	838	845	854	rVV	70837	211071	10.32%	1.923%
16	6.336	854	861	875	rVB5	19423	69906	3.42%	0.637%
17	6.763	920	931	950	rBV	202929	480117	23.47%	4.374%
18	7.379	1022	1032	1042	rBV3	17082	41171	2.01%	0.375%
19	7.665	1073	1079	1092	rBV2	11384	25810	1.26%	0.235%
20	8.427	1193	1204	1212	rBV	60011	107285	5.24%	0.977%
21	8.647	1235	1240	1249	rVB	406093	642118	31.39%	5.850%
22	9.006	1295	1299	1304	rVB	26551	37559	1.84%	0.342%
23	9.171	1322	1326	1332	rVB	15986	23883	1.17%	0.218%
24	9.244	1332	1338	1343	rBV	20522	30699	1.50%	0.280%
25	9.494	1374	1379	1388	rVB	55304	89392	4.37%	0.814%
26	9.945	1448	1453	1460	rBV	22354	34143	1.67%	0.311%
27	10.055	1465	1471	1480	rVV	411444	611982	29.92%	5.576%
28	10.311	1505	1513	1520	rVB3	35427	67505	3.30%	0.615%
29	10.963	1613	1620	1625	rBV	76420	95563	4.67%	0.871%
30	11.079	1634	1639	1644	rBV	314443	418499	20.46%	3.813%
31	11.122	1644	1646	1651	rVV	29657	34237	1.67%	0.312%
32	11.616	1723	1727	1734	rBV3	14644	28455	1.39%	0.259%
33	11.744	1745	1748	1755	rVB	40474	55617	2.72%	0.507%
34	11.841	1755	1764	1766	rBV	16805	26567	1.30%	0.242%
35	11.890	1768	1772	1775	rVB	26843	35606	1.74%	0.324%
36	11.933	1775	1779	1783	rBV	82689	99950	4.89%	0.911%

LSC Area Percent Report

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Integrator: RTE
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Title : SW846 8260

37	12.024	1789	1794	1799	rBV	391630	494827	24.19%	4.508%
38	12.128	1805	1811	1812	rBV	45783	61823	3.02%	0.563%
39	12.146	1812	1814	1818	rVB	49508	59206	2.89%	0.539%
40	12.244	1825	1830	1836	rBV2	159364	215786	10.55%	1.966%
41	12.305	1836	1840	1843	rBV3	23476	38489	1.88%	0.351%
42	12.616	1886	1891	1894	rBV	100710	125371	6.13%	1.142%
43	12.701	1901	1905	1916	rVB3	31763	57160	2.79%	0.521%
44	12.920	1934	1941	1946	rBV	100578	134814	6.59%	1.228%
45	13.024	1952	1958	1966	rVB3	15537	24017	1.17%	0.219%
46	13.122	1971	1974	1979	rVV5	15106	28626	1.40%	0.261%
47	13.170	1979	1982	1990	rVB	19846	25818	1.26%	0.235%
48	13.292	1998	2002	2008	rVV3	34330	65908	3.22%	0.600%
49	13.579	2046	2049	2055	rVB2	19302	23228	1.14%	0.212%

Sum of corrected areas: 10976073

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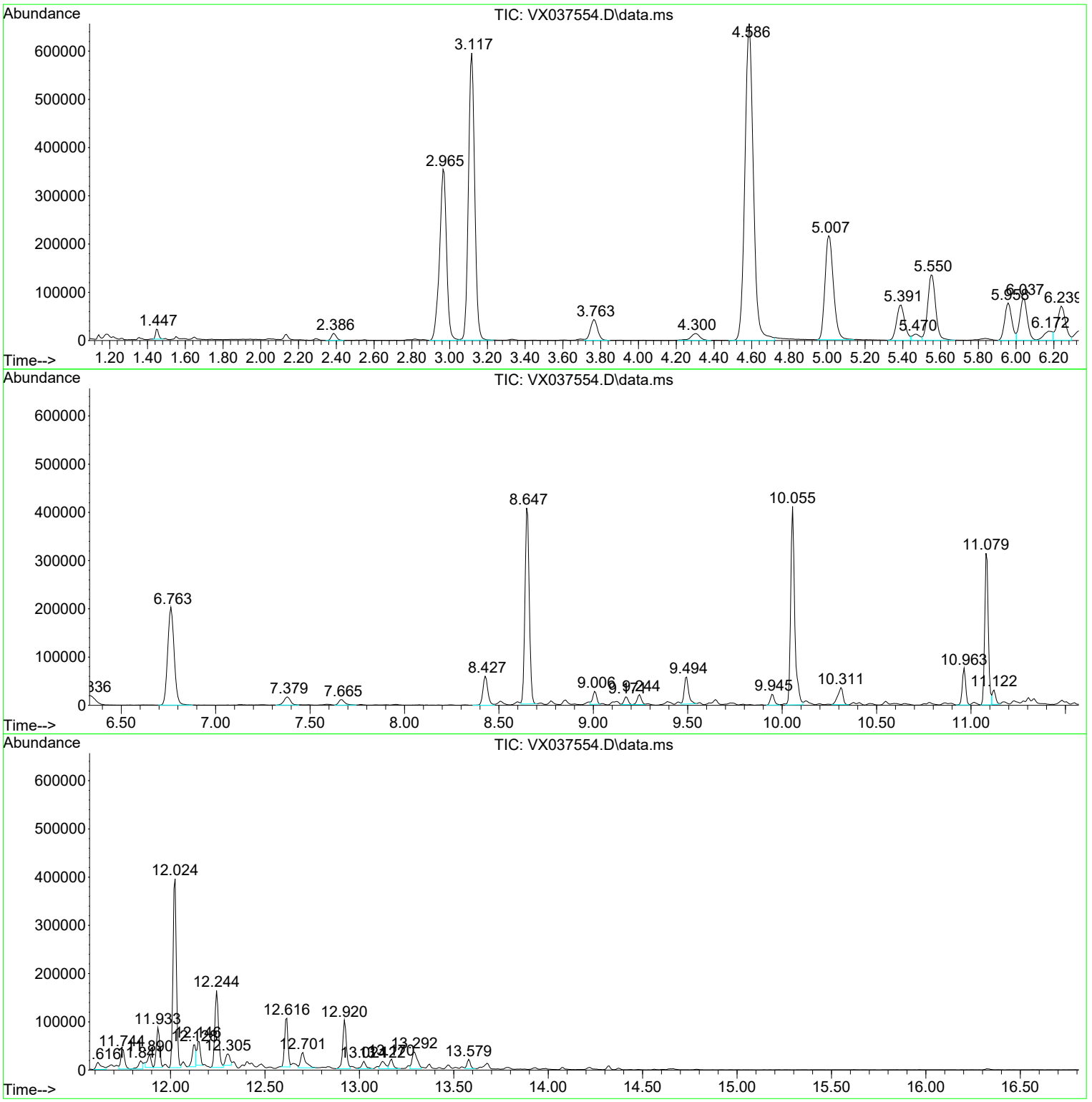
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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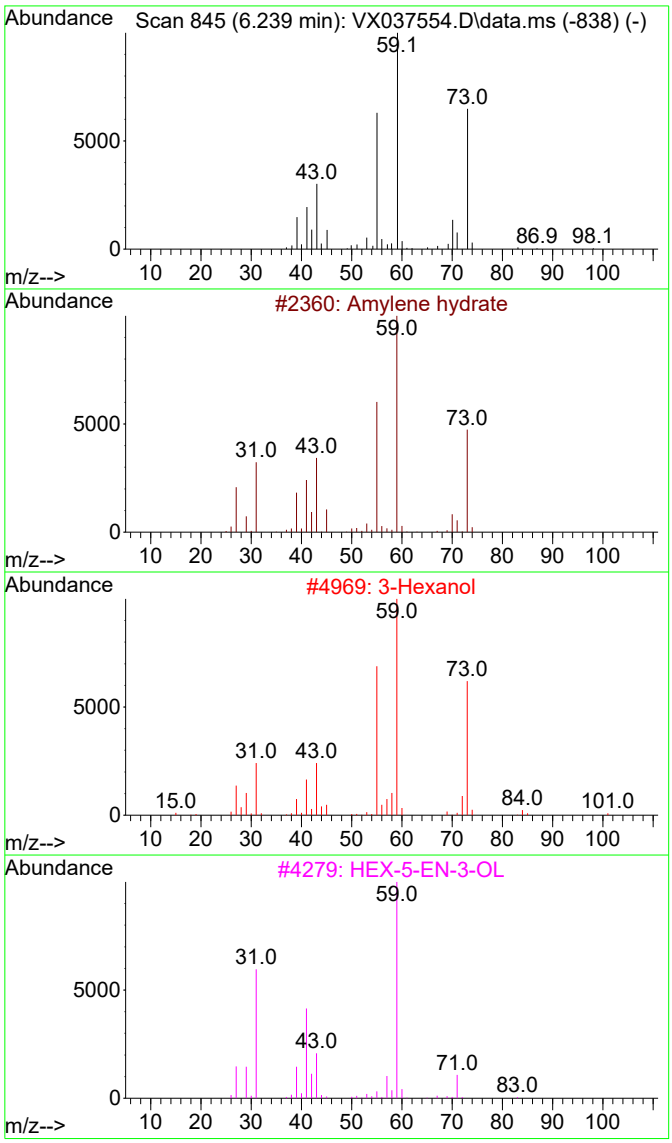
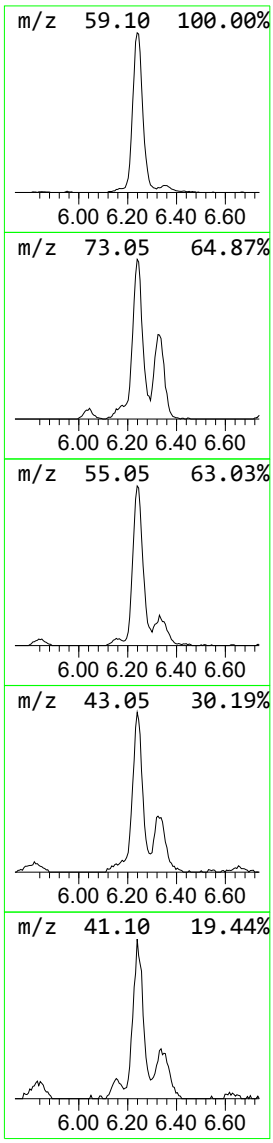
****

Peak Number 3 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	21.98 ug/l	211071	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	83
2	3-Hexanol	102	C6H14O	000623-37-0	45
3	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	42
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	40
5	Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	28





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Data File : VX037554.D
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Instrument :
MSVOA_X
ClientSampleId :
MW5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

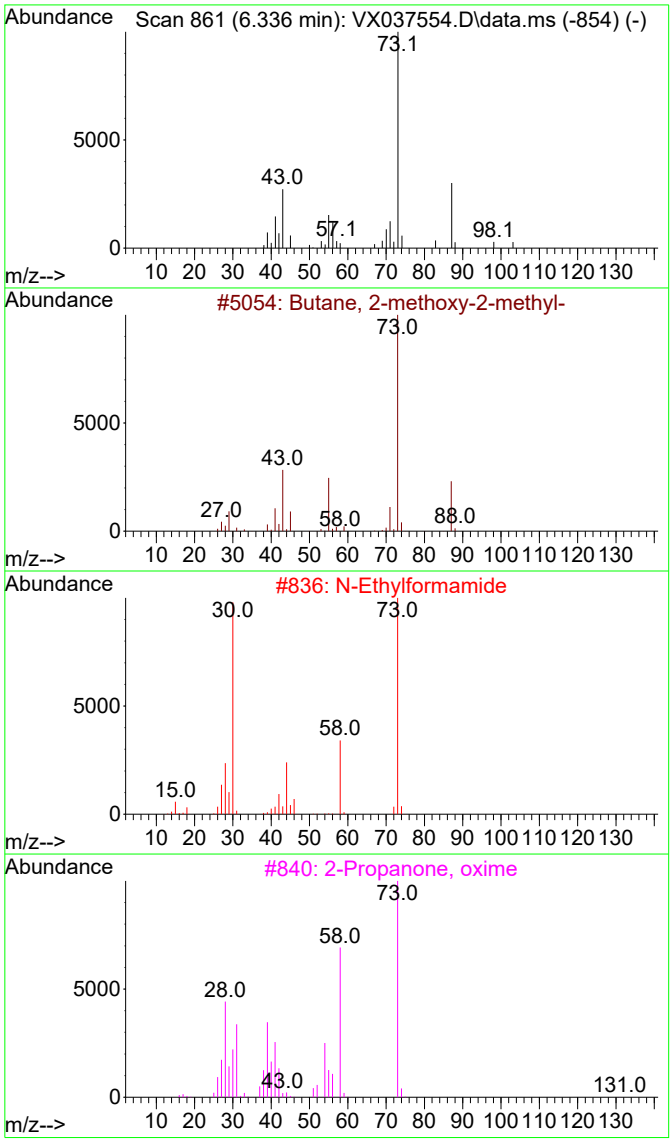
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

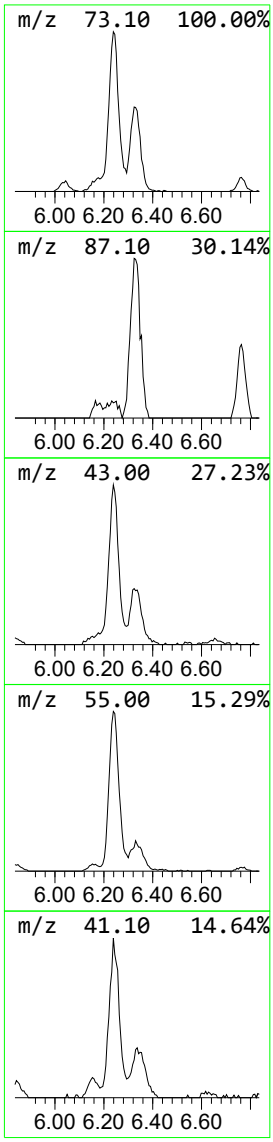
****

Peak Number 4 unknown6.336 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.336	7.28 ug/l	69906	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	42
2	N-Ethylformamide	73	C3H7NO	000627-45-2	12
3	2-Propanone, oxime	73	C3H7NO	000127-06-0	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

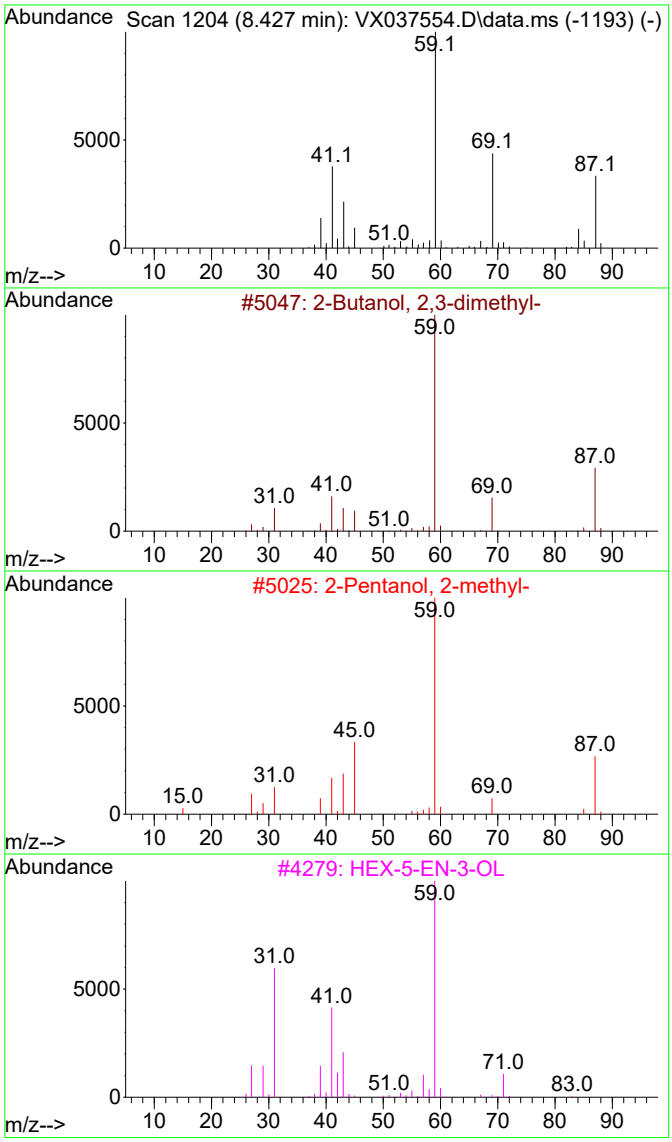
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

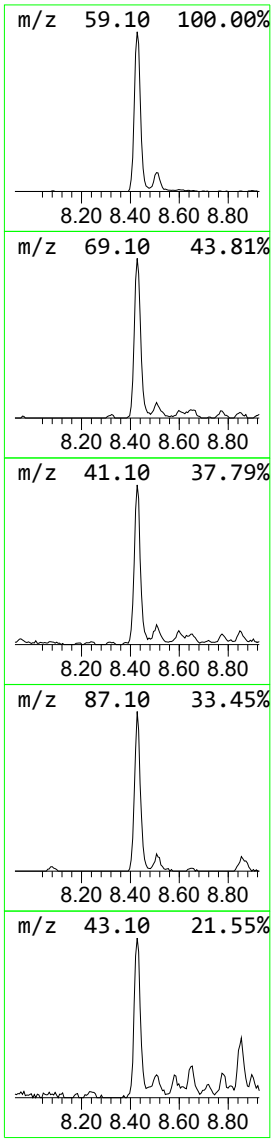
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanol, 2,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.427	8.77 ug/l	107285	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	50
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	45
5	3-Heptanol	116	C7H16O	000589-82-2	39





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Instrument :
MSVOA_X
ClientSampleId :
MW5

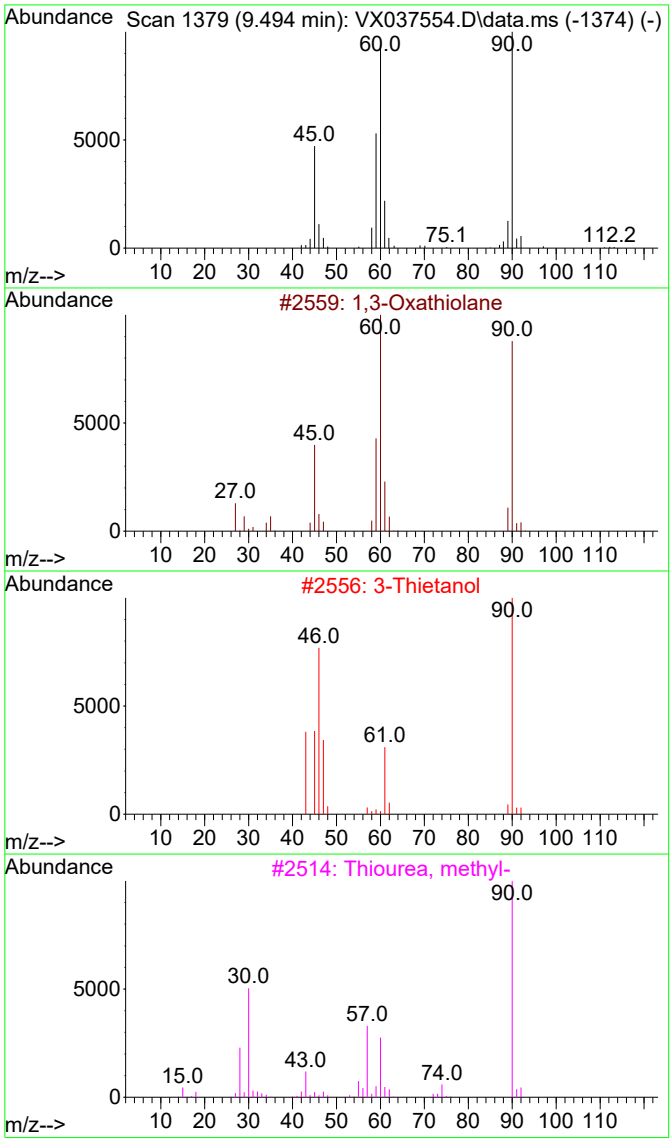
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

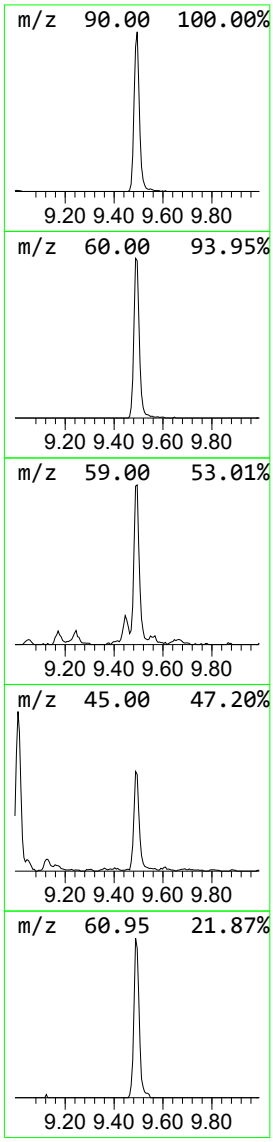
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Oxathiolane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.494	7.30 ug/l	89392	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Oxathiolane	90	C3H6OS	002094-97-5	94
2	3-Thietanol	90	C3H6OS	010304-16-2	53
3	Thiourea, methyl-	90	C2H6N2S	000598-52-7	50
4	(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	33
5	Thiazole, 4,5-dihydro-2-methyl-	101	C4H7NS	002346-00-1	14





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Instrument :
MSVOA_X
ClientSampleId :
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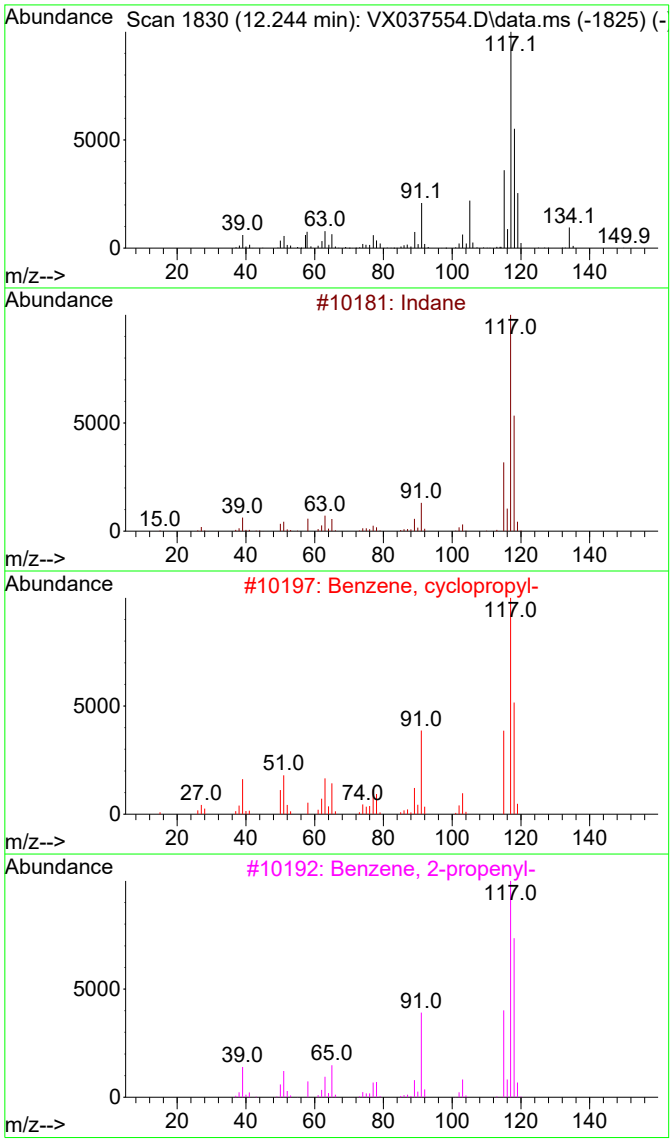
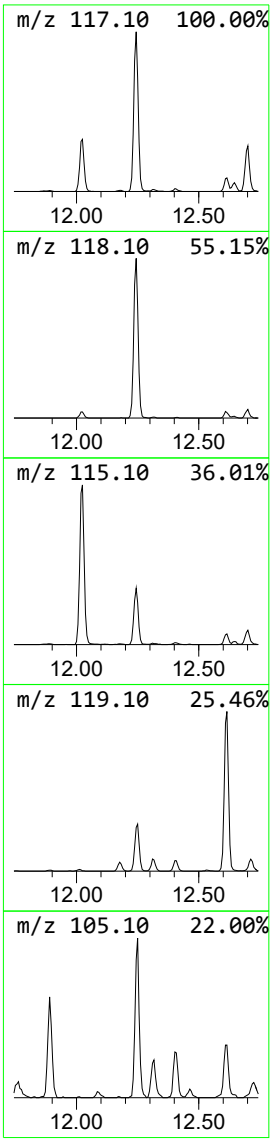
****
Peak Number 7 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	21.80 ug/l	215786	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, cyclopropyl-	118	C9H10	000873-49-4	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	58





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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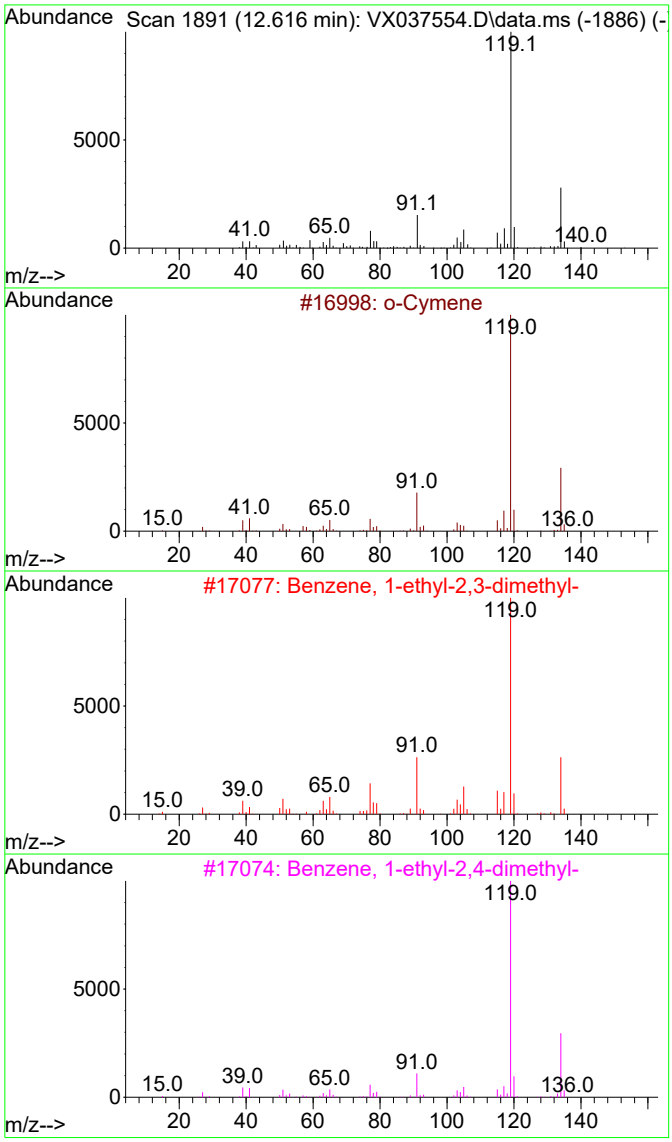
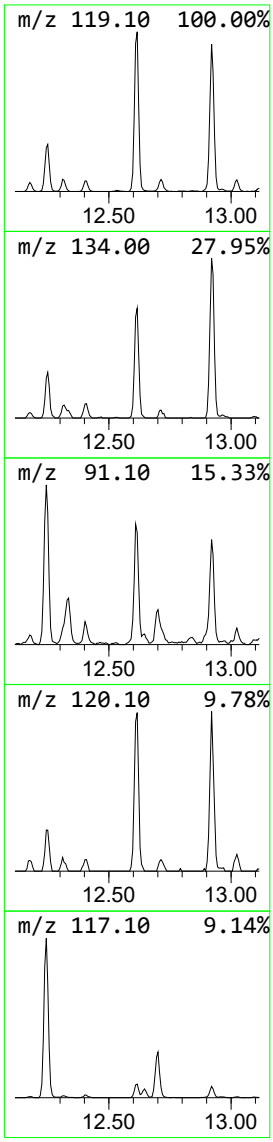
****

Peak Number 8 o-Cymene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	12.67 ug/l	125371	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	o-Cymene	134	C10H14	000527-84-4	97
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	96
3	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
5	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94





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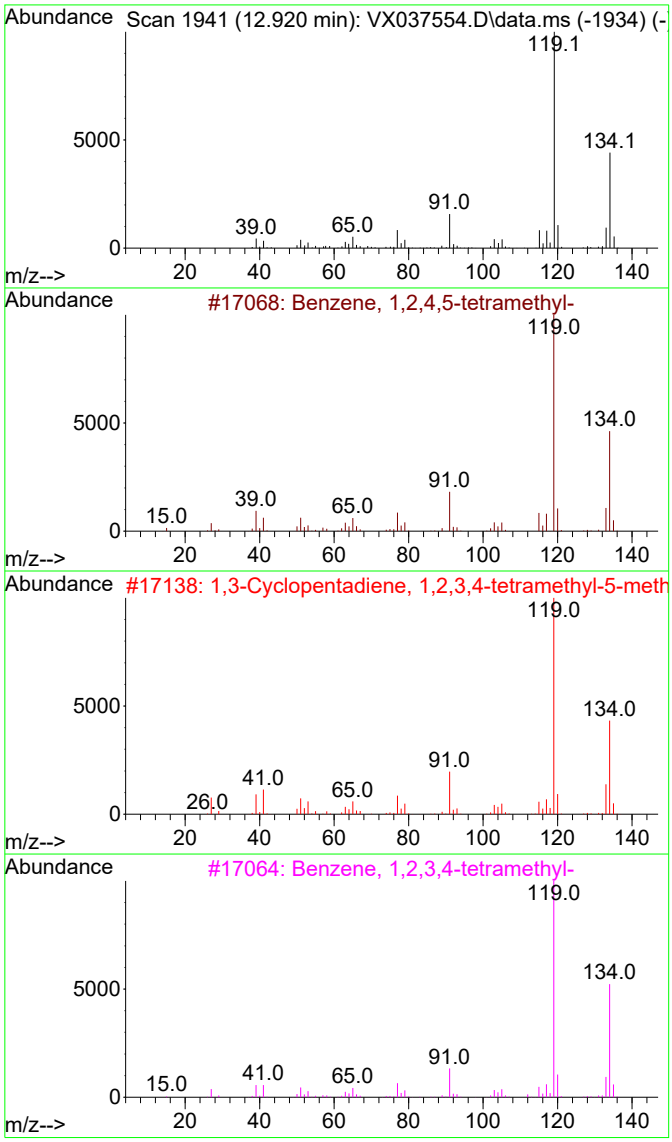
Quant Title : SW846 8260

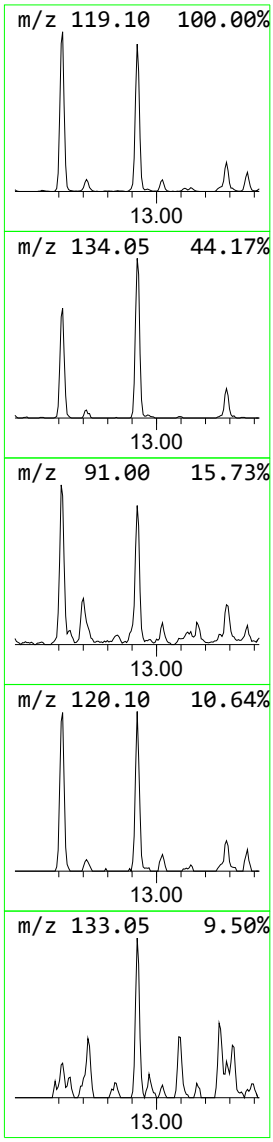
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	13.62 ug/l	134814	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	97
3	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
4	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
5	o-Cymene	134	C10H14	000527-84-4	94





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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
MW5

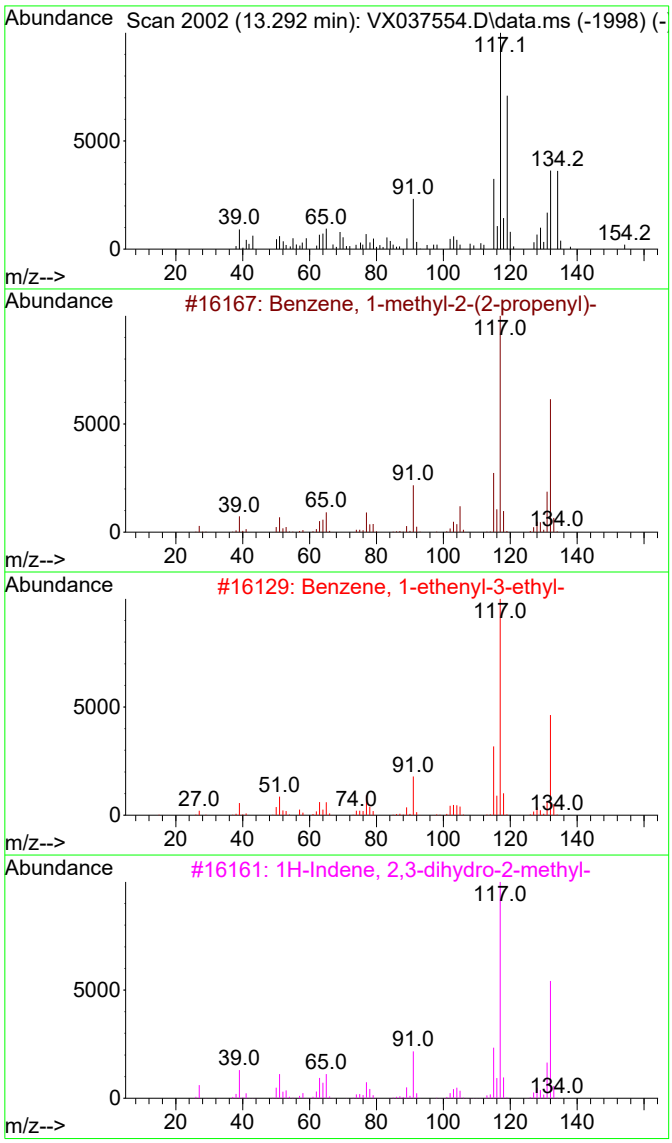
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

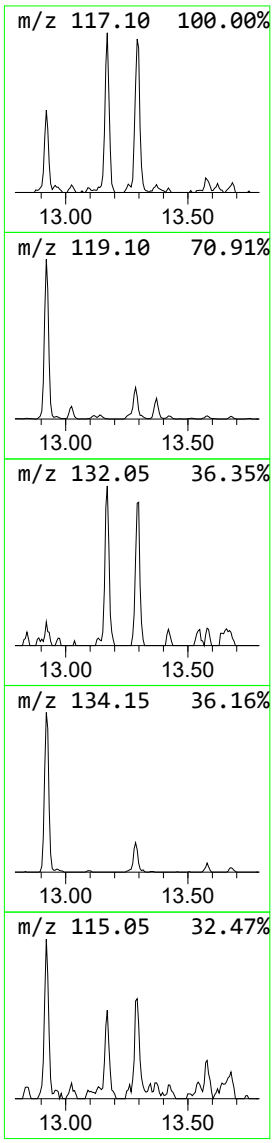
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-methyl-2-(2-prop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	6.66 ug/l	65908	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	64
3	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	60
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	58
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090623\
Data File : VX037554.D
Acq On : 06 Sep 2023 15:00
Operator : JC/MD
Sample : 04220-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.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
Amylene hydrate	6.239	22.0	ug/l	211071	2	6.763	480117	50.0
unknown6.336	6.336	7.3	ug/l	69906	2	6.763	480117	50.0
2-Butanol, 2,3-...	8.427	8.8	ug/l	107285	3	10.055	611982	50.0
1,3-Oxathiolane	9.494	7.3	ug/l	89392	3	10.055	611982	50.0
Indane	12.244	21.8	ug/l	215786	4	12.024	494827	50.0
o-Cymene	12.616	12.7	ug/l	125371	4	12.024	494827	50.0
Benzene, 1,2,4,...	12.920	13.6	ug/l	134814	4	12.024	494827	50.0
Benzene, 1-meth...	13.292	6.7	ug/l	65908	4	12.024	494827	50.0