

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX020420\
 Data File : VX014806.D
 Acq On : 04 Feb 2020 14:02
 Operator : JC/SP
 Sample : L1388-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TOTE-COMP

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	44	rBV	552913	733227	1.87%	0.937%
2	5.490	742	755	765	rBV	237766	691989	1.77%	0.884%
3	5.654	771	782	794	rVB	413294	1148963	2.93%	1.468%
4	6.051	838	847	858	rBV	268054	678957	1.73%	0.867%
5	6.849	968	978	990	rBV	658129	1571331	4.01%	2.007%
6	8.709	1277	1283	1290	rBV	1387320	2090471	5.34%	2.670%
7	10.105	1507	1512	1522	rVB	1340653	1830561	4.67%	2.338%
8	11.135	1675	1681	1687	rBV	1097704	1433868	3.66%	1.831%
9	12.074	1830	1835	1842	rVB	1569818	1903617	4.86%	2.431%
10	12.263	1861	1866	1869	rBV	3130682	3838136	9.80%	4.902%
11	12.294	1869	1871	1879	rVB	1735228	1904323	4.86%	2.432%
12	12.464	1892	1899	1904	rBV	1106316	1356566	3.46%	1.733%
13	13.830	2118	2123	2129	rVB	29393454	39161922	100.00%	50.021%
14	13.921	2134	2138	2143	rBV	1194695	1382662	3.53%	1.766%
15	14.689	2260	2264	2274	rVB	6078648	7153856	18.27%	9.138%
16	14.836	2282	2288	2297	rVB	3194164	4047750	10.34%	5.170%
17	15.263	2350	2358	2364	rBV	890183	1229080	3.14%	1.570%
18	15.543	2397	2404	2409	rBV	331168	519473	1.33%	0.664%
19	15.683	2418	2427	2430	rBV	372832	630778	1.61%	0.806%
20	16.409	2537	2546	2555	rBV	2486475	4312276	11.01%	5.508%
21	16.774	2597	2606	2608	rBV	372811	671341	1.71%	0.857%

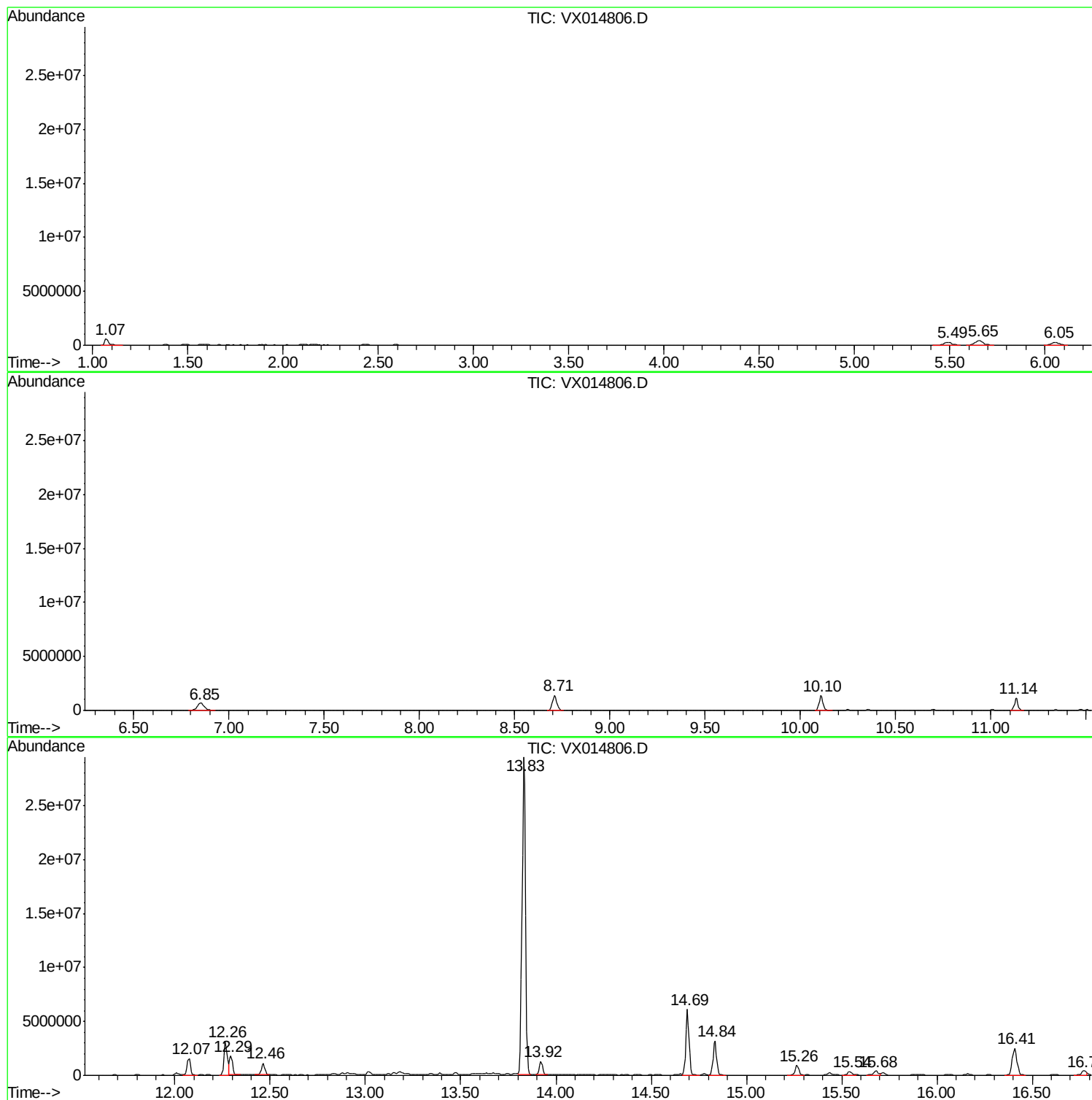
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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



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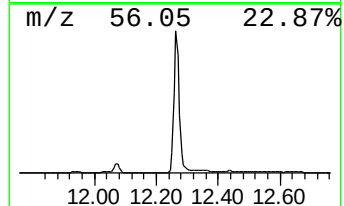
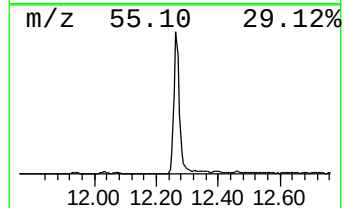
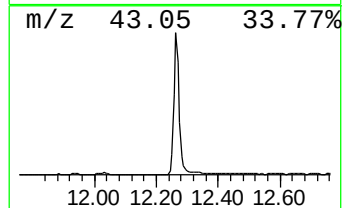
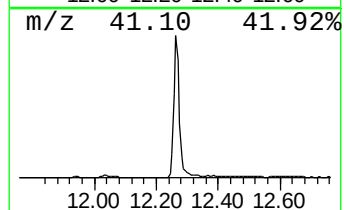
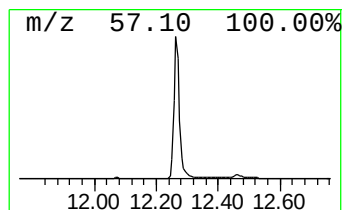
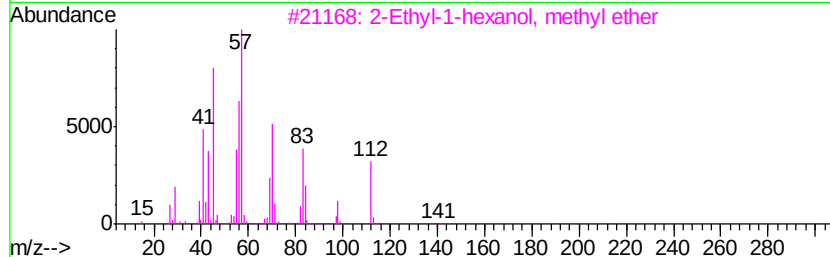
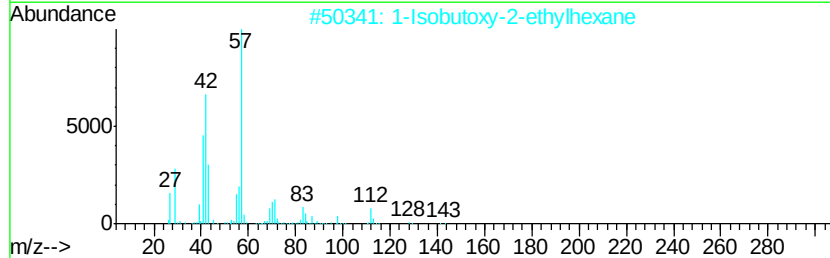
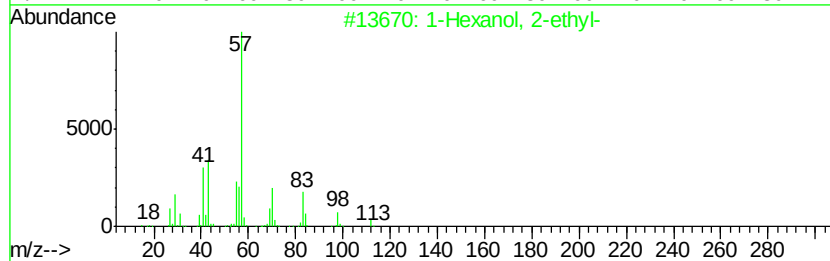
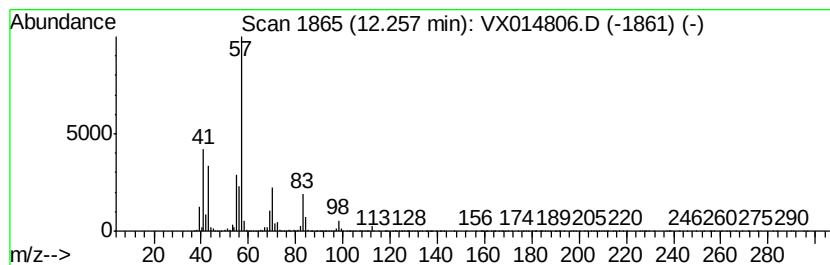
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	100.81 ug/l	3838140	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42



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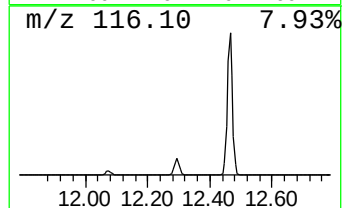
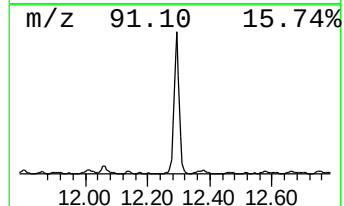
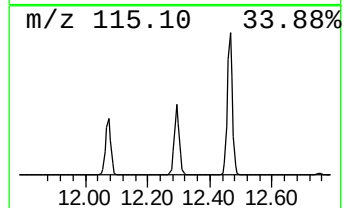
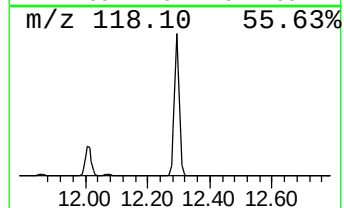
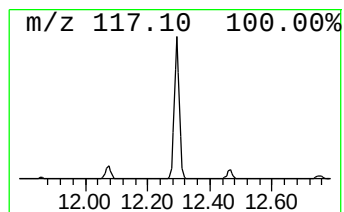
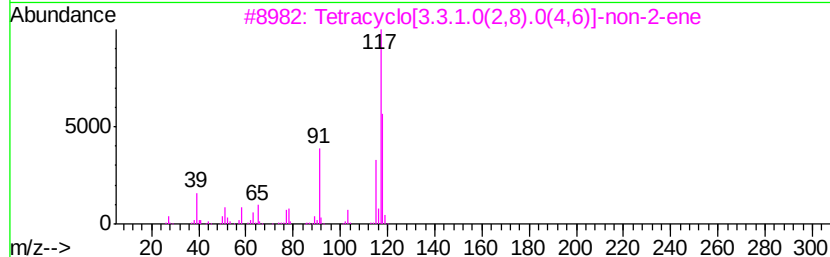
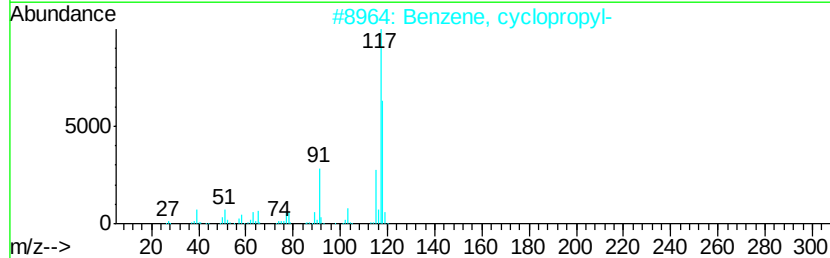
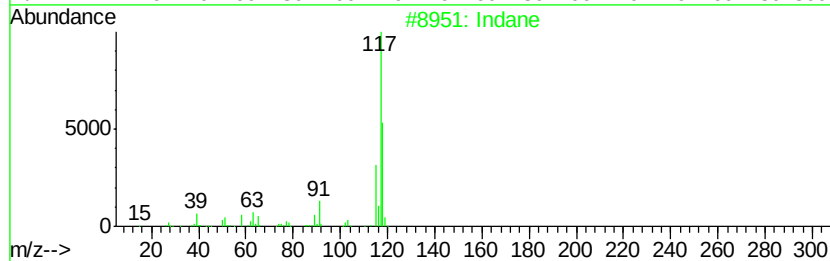
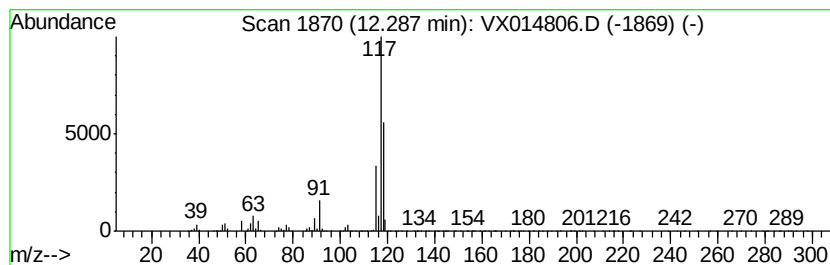
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Quant Title : SW846 8260

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

Peak Number 3 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	50.02 ug/l	1904320	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-		118	C9H10	000873-49-4	83
3	Tetracyclo[3.3.1.0(2,8).0(4,6)]-	...	118	C9H10	1000191-13-7	80
4	Deltacyclene		118	C9H10	007785-10-6	80
5	Benzene, 1-propenyl-		118	C9H10	000637-50-3	72



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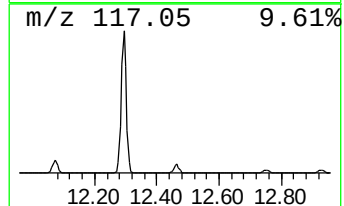
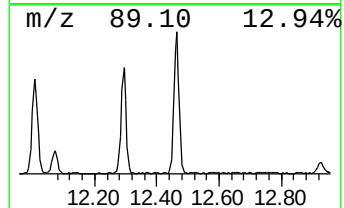
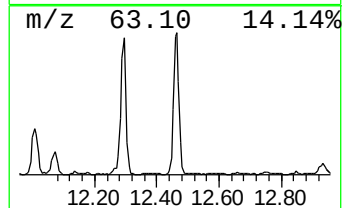
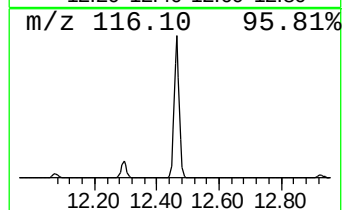
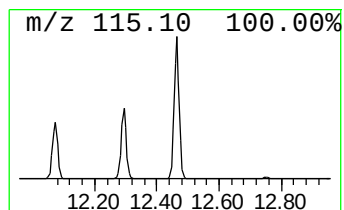
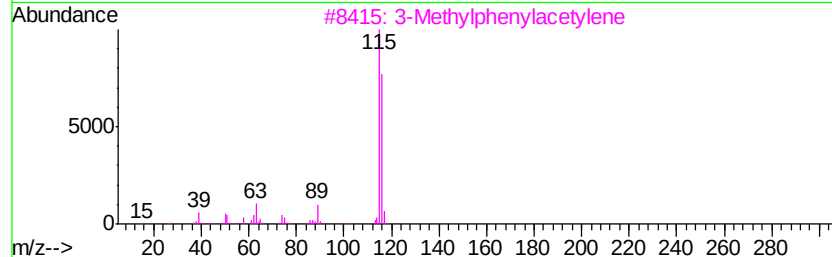
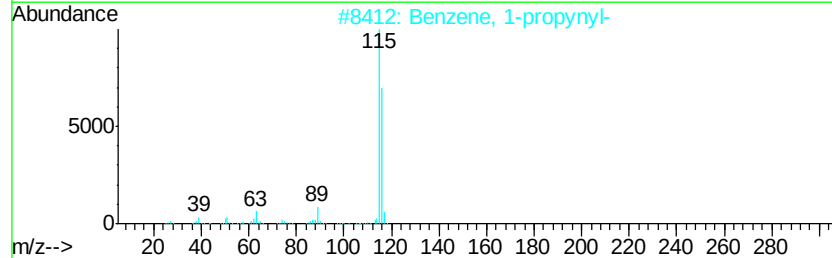
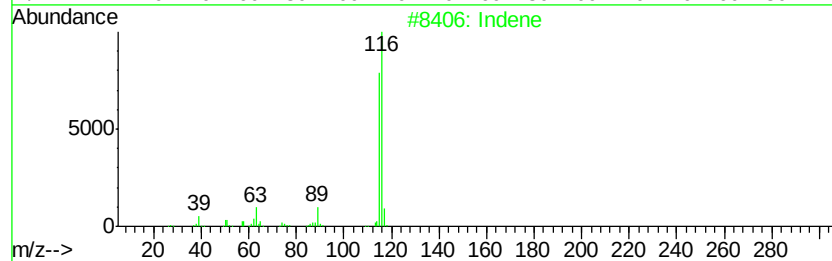
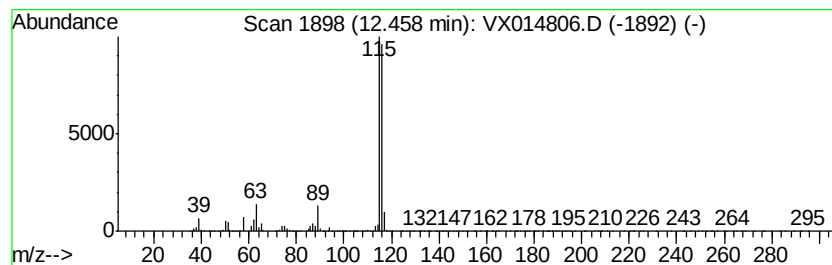
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Peak Number 4 Indene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	35.63 ug/l	1356570	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene		116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-		116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene		116	C9H8	000766-82-5	91
4	2-Methylphenylacetylene		116	C9H8	000766-47-2	91
5	Benzene, 1-ethynyl-4-methyl-		116	C9H8	000766-97-2	90



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
TOTE-COMP

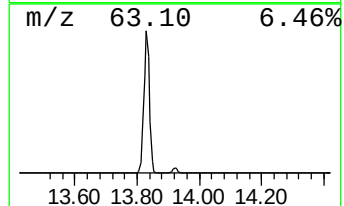
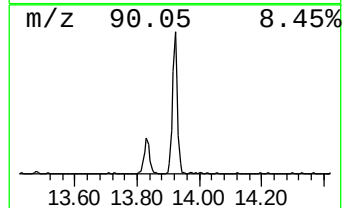
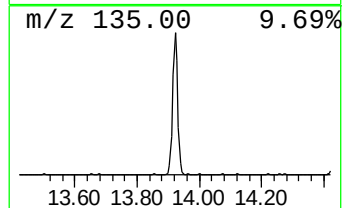
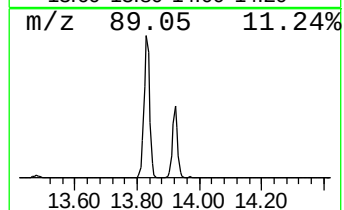
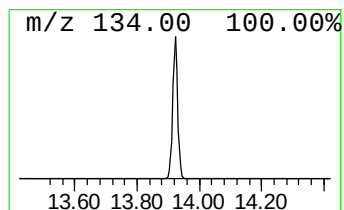
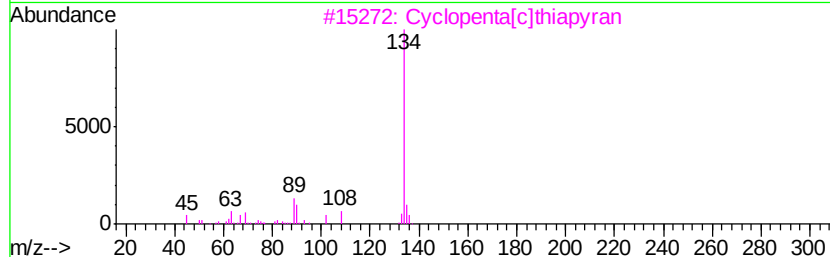
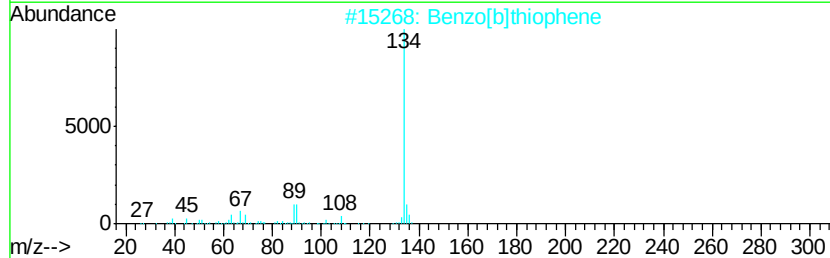
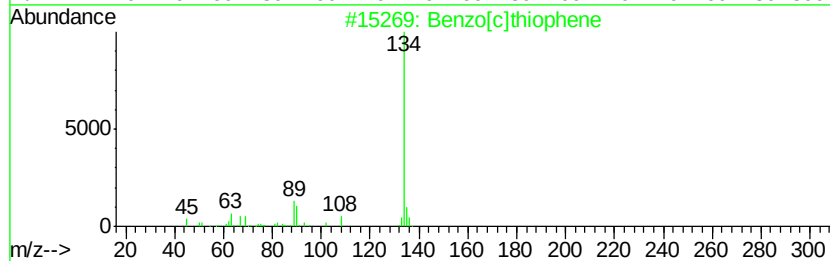
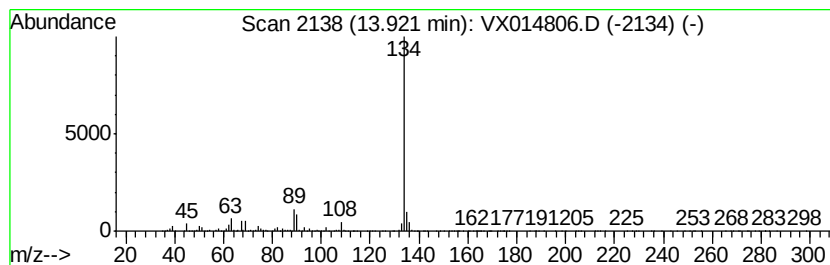
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Quant Title : SW846 8260

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

Peak Number 5 Benzo[c]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	36.32 ug/l	1382660	1,4-Dichlorobenzene-d4	12.07

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	97
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	94
3	Cyclopenta[c]thiopyran	134	C8H6S	000270-63-3	94
4	[1]Benzo[thieno[2',3':3,4]cyclobu...	246	C13H10O3S	034002-19-2	64
5	Thiazolidin-4-one, 5-benzylideno...	287	C13H9N3OS2	351062-07-2	45



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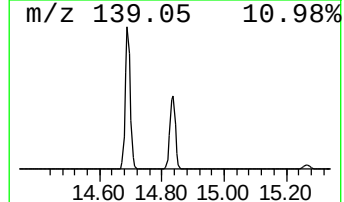
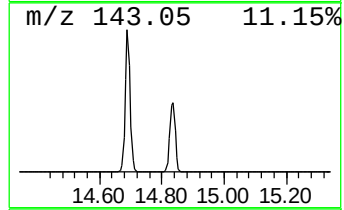
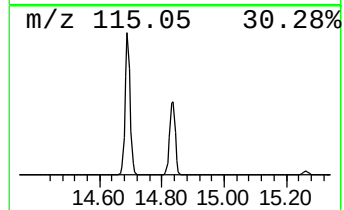
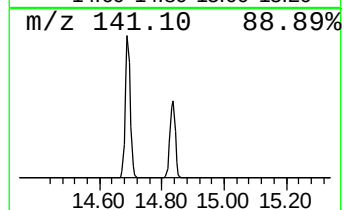
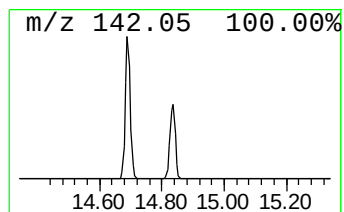
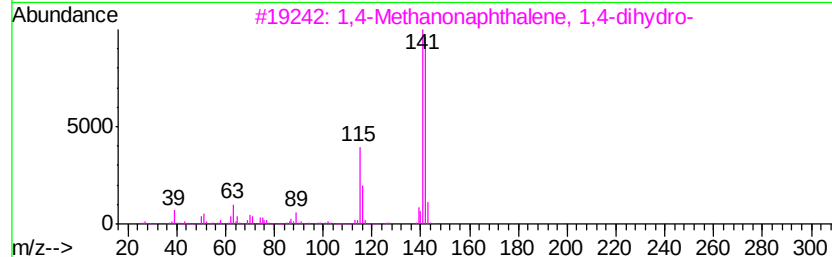
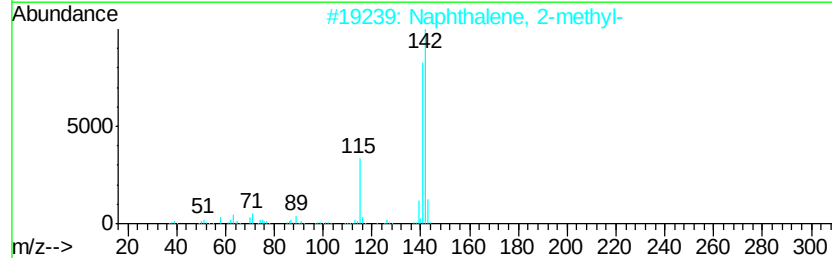
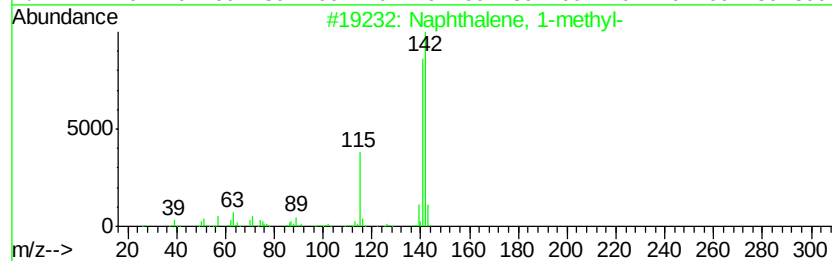
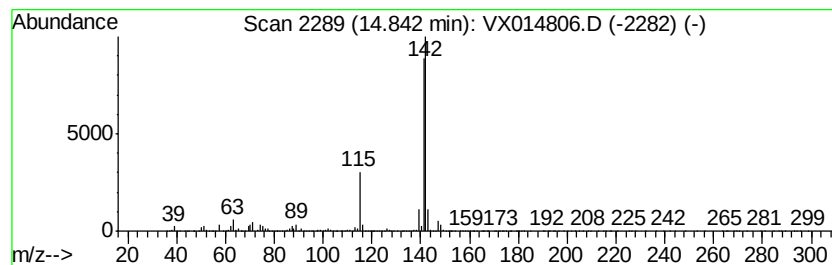
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	106.32 ug/l	4047750	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-ethyl-	12.26	100.8	ug/l	3838140	4	12.07	1903620	50.0
Indane	12.29	50.0	ug/l	1904320	4	12.07	1903620	50.0
Indene	12.46	35.6	ug/l	1356570	4	12.07	1903620	50.0
Benzo[c]thiophene	13.92	36.3	ug/l	1382660	4	12.07	1903620	50.0
Naphthalene, 1-me...	14.84	106.3	ug/l	4047750	4	12.07	1903620	50.0