

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
 Data File : VX040325.D
 Acq On : 19 Feb 2024 13:07
 Operator : JC/MD
 Sample : P1395-03 40X
 Misc : 3.46g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-2(4-6)

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\82X020924W.M
 Title : SW846 8260

Signal : TIC: VX040325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.379	694	704	718	rBV2	53690	157162	1.26%	0.753%
2	5.550	721	732	750	rVB2	89518	258479	2.07%	1.239%
3	5.952	789	798	805	rBV	63004	166402	1.34%	0.798%
4	6.757	921	930	945	rBV	145236	351748	2.82%	1.686%
5	7.123	981	990	1002	rBV2	88091	195824	1.57%	0.939%
6	8.647	1234	1240	1245	rBV	307677	484370	3.89%	2.322%
7	8.720	1245	1252	1267	rVB	7700936	12461003	100.00%	59.731%
8	10.055	1465	1471	1472	rBV	338261	458480	3.68%	2.198%
9	10.080	1472	1475	1488	rVB	635179	845463	6.78%	4.053%
10	10.189	1488	1493	1504	rVB	174573	241585	1.94%	1.158%
11	10.299	1504	1511	1518	rBV	792315	1060630	8.51%	5.084%
12	10.640	1561	1567	1583	rVB2	236516	375071	3.01%	1.798%
13	11.079	1634	1639	1651	rVB	284486	362549	2.91%	1.738%
14	11.835	1758	1763	1769	rBV	153034	183566	1.47%	0.880%
15	12.018	1788	1793	1809	rVB3	393137	851317	6.83%	4.081%
16	13.420	2018	2023	2026	rBV	137710	162569	1.30%	0.779%
17	13.774	2076	2081	2091	rBV	104255	129479	1.04%	0.621%
18	15.207	2309	2316	2326	rBV	333730	470811	3.78%	2.257%
19	15.322	2329	2335	2341	rBV	808293	1109526	8.90%	5.318%
20	16.060	2449	2456	2464	rBV	335763	535855	4.30%	2.569%

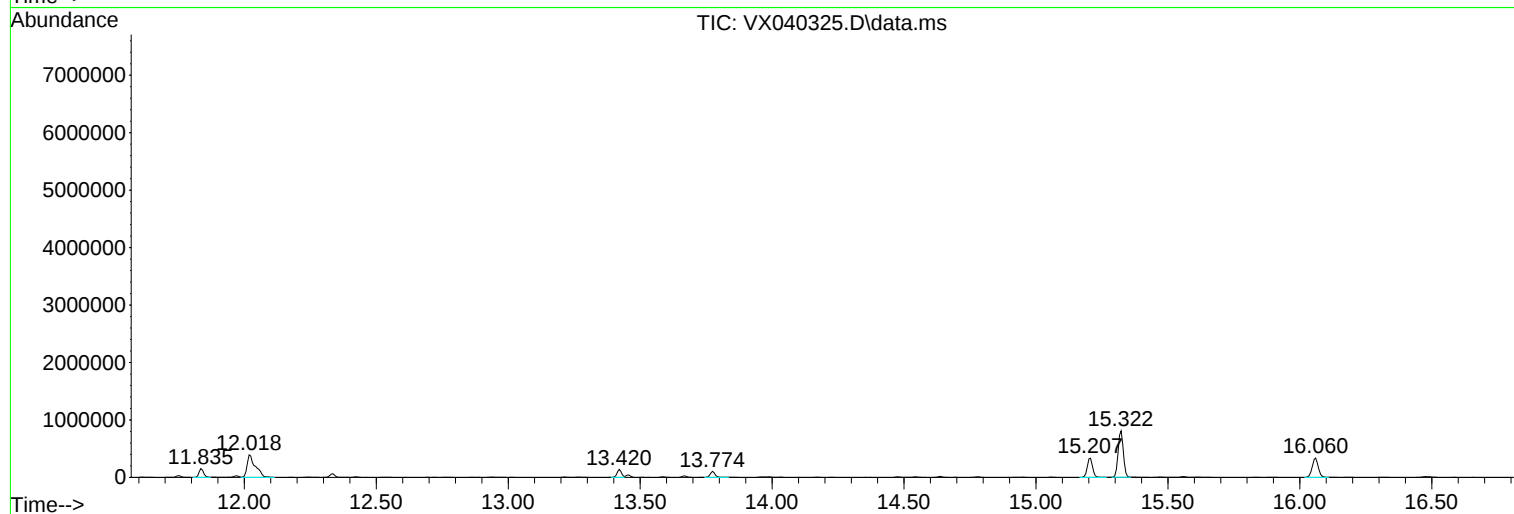
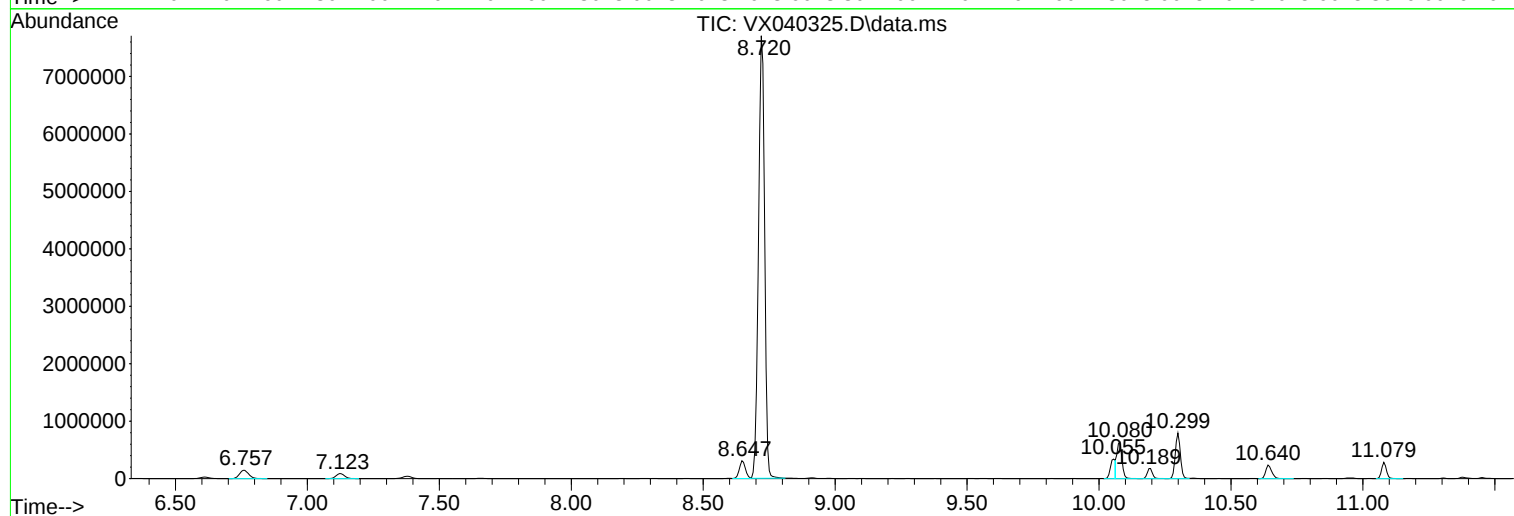
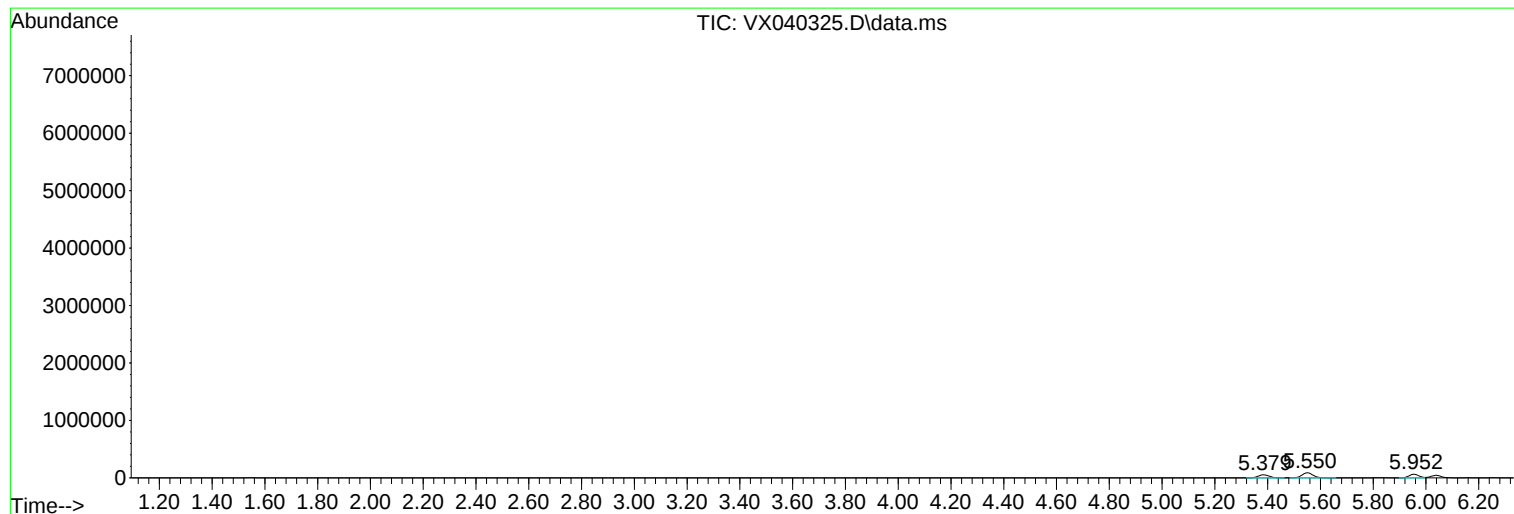
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B-2(4-6)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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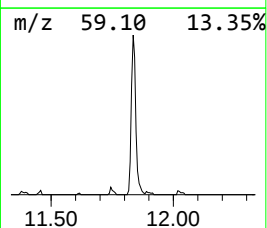
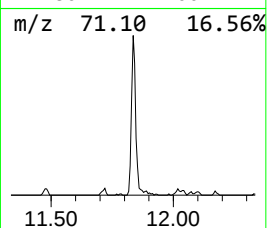
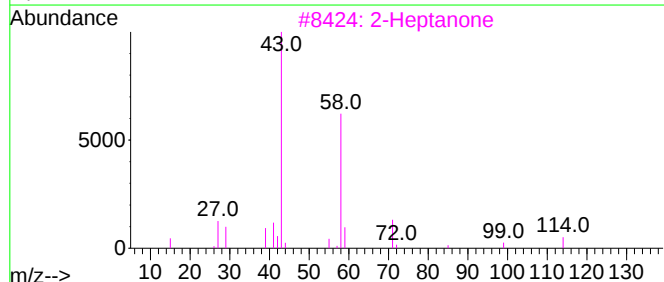
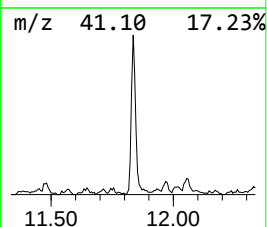
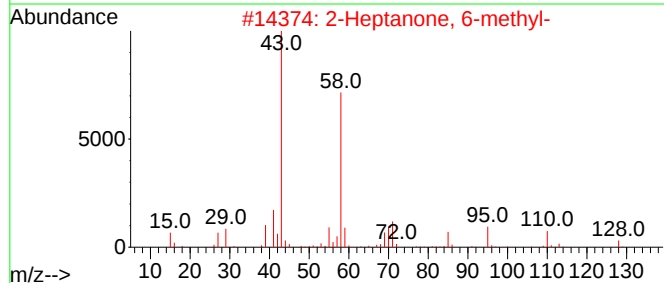
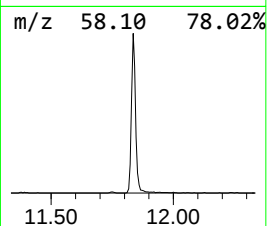
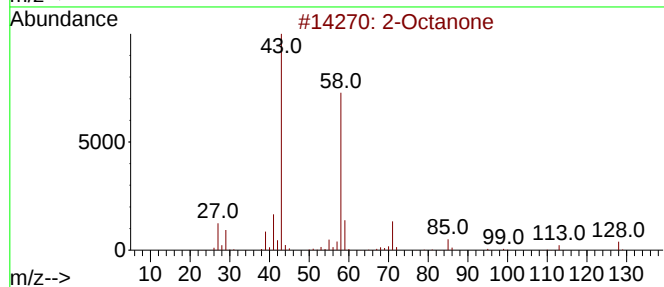
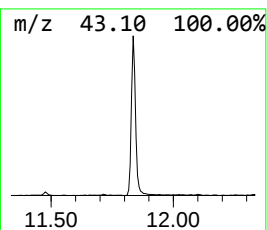
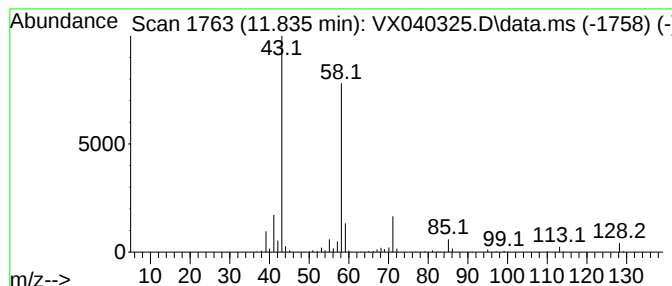
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.835	10.78 ug/l	183566	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	94
2			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	90
3			2-Heptanone	114	C7H14O	000110-43-0	72
4			2-Butoxy-N-(2-(dimethylamino)eth...	315	C18H25N3O2	1000425-82-7	53
5			Propanal	58	C3H6O	000123-38-6	40



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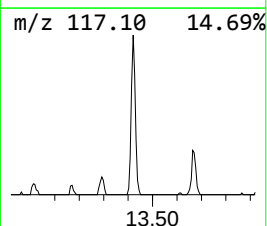
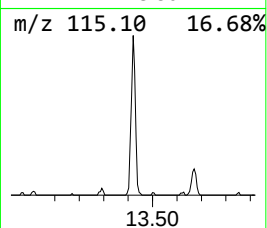
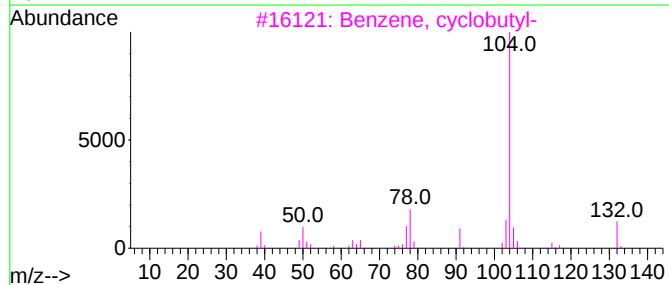
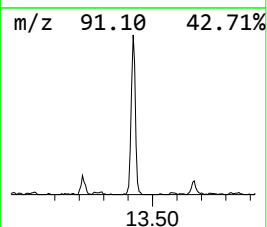
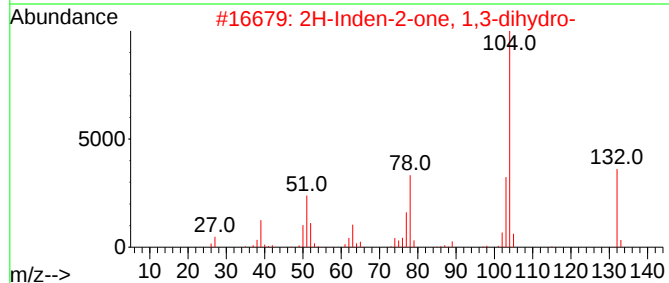
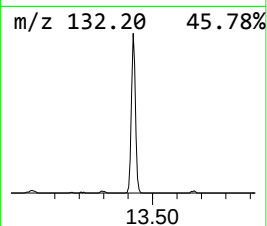
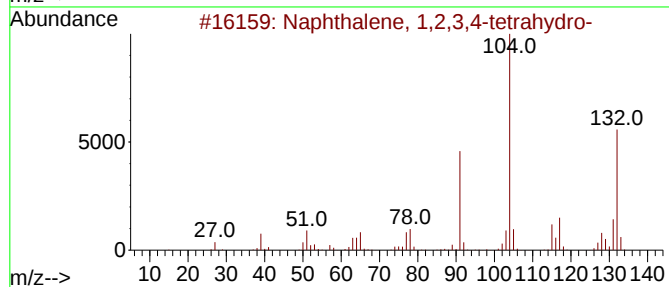
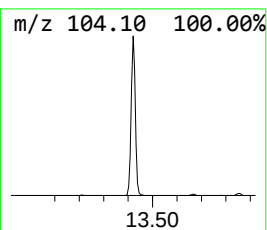
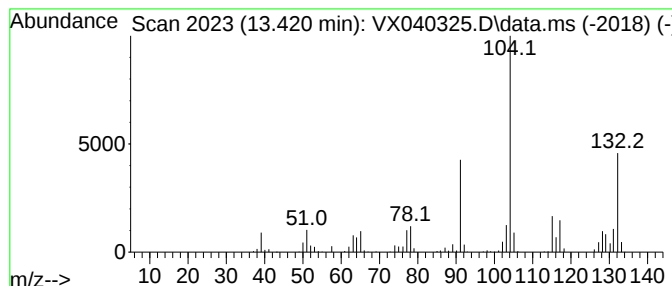
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Quant Title : SW846 8260

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Peak Number 2 Naphthalene, 1,2,3,4-tetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.420	9.55 ug/l	162569	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	58
3			Benzene, cyclobutyl-	132	C10H12	004392-30-7	53
4			Indan, epoxide	132	C9H8O	000768-22-9	52
5			2-Methylbenzyl cyanide	131	C9H9N	022364-68-7	49



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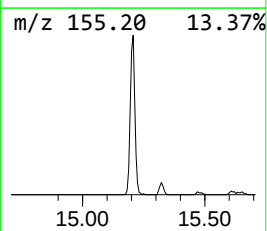
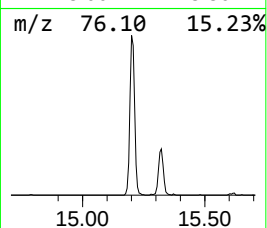
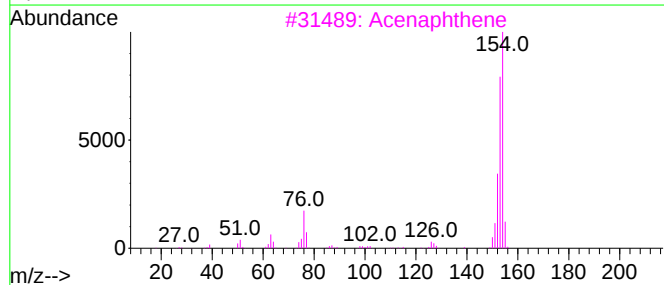
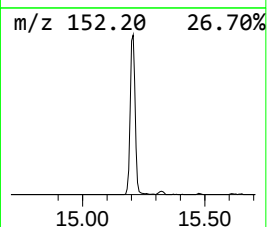
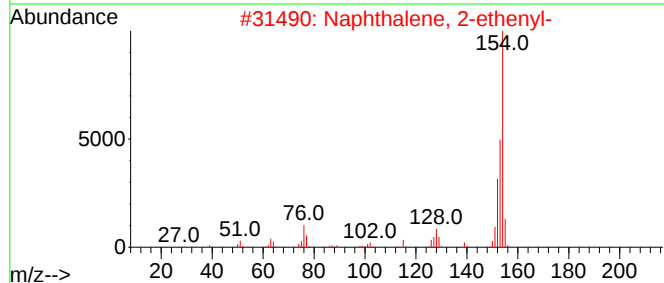
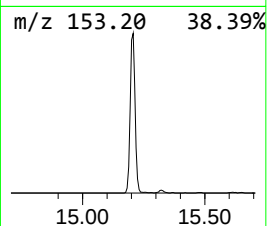
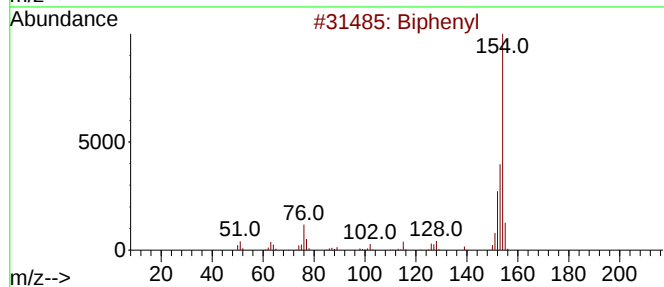
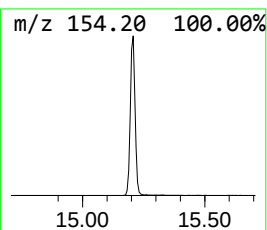
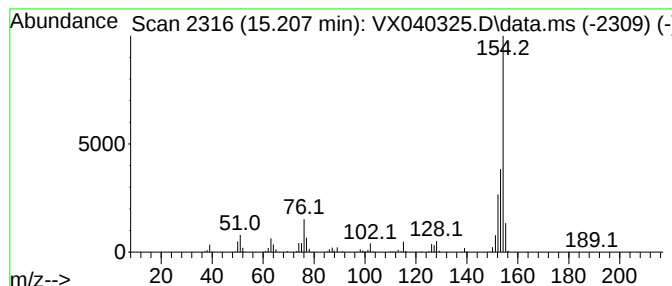
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, 2-ethenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	27.65 ug/l	470811	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	95
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	87
3			Acenaphthene	154	C12H10	000083-32-9	49
4			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	45
5			6-Cyanoquinoline	154	C10H6N2	023395-72-4	43



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ClientSampleId :
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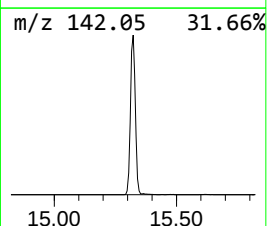
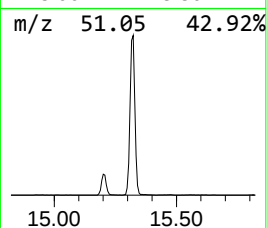
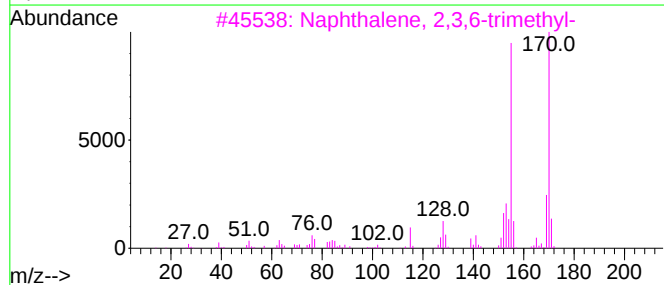
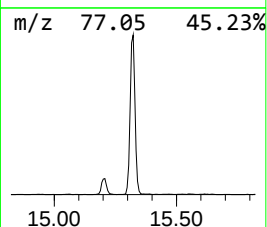
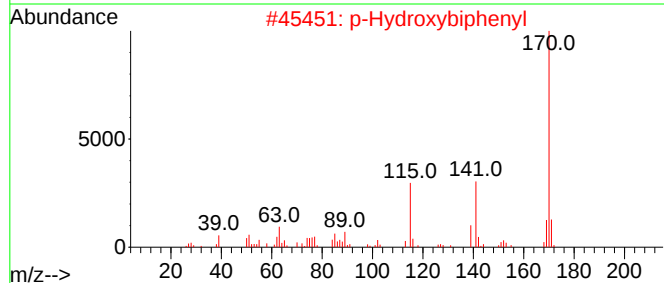
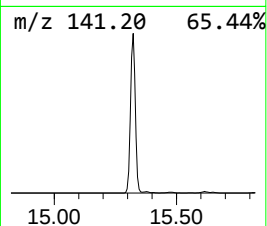
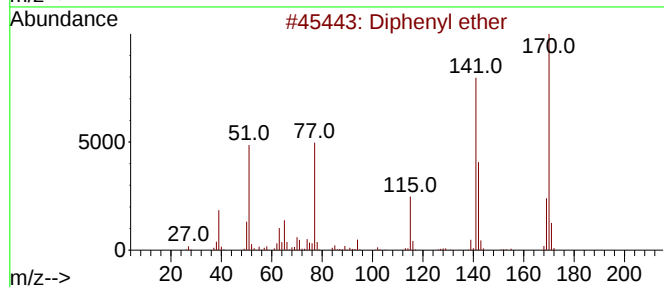
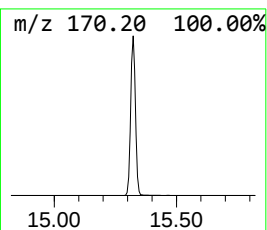
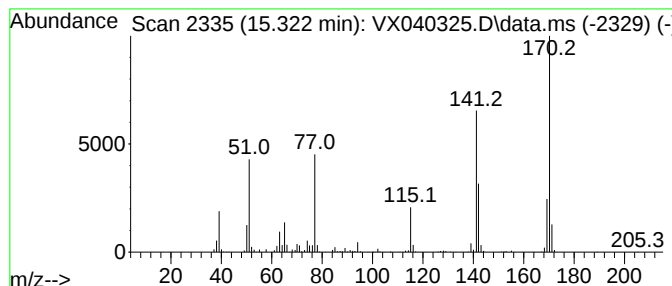
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Diphenyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.323	65.17 ug/l	1109530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diphenyl ether	170	C12H10O	000101-84-8	98
2			p-Hydroxybiphenyl	170	C12H10O	000092-69-3	38
3			Naphthalene, 2,3,6-trimethyl-	170	C13H14	000829-26-5	35
4			o-Hydroxybiphenyl	170	C12H10O	000090-43-7	32
5			Phenol, O-(ethylsulfinyl)-	170	C8H10O2S	029634-40-0	32



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ClientSampleId :
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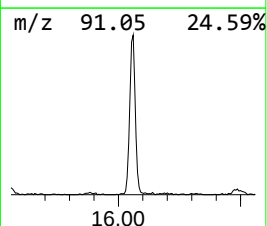
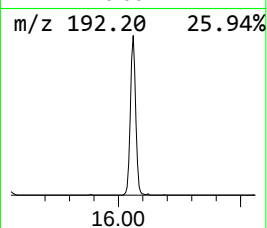
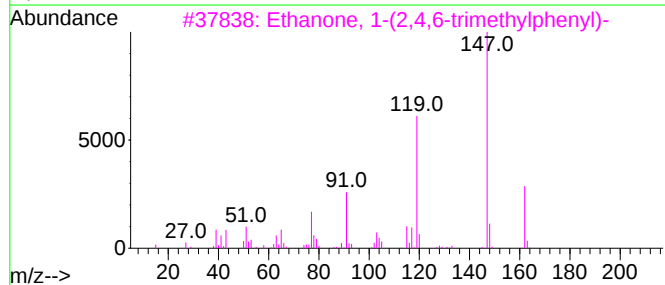
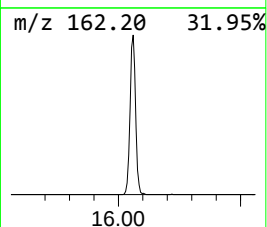
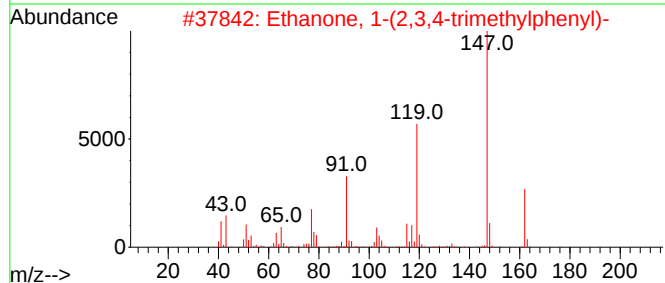
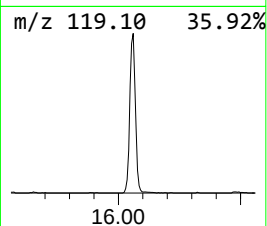
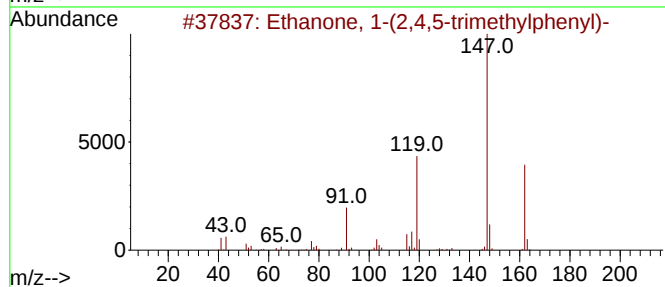
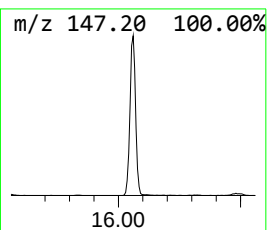
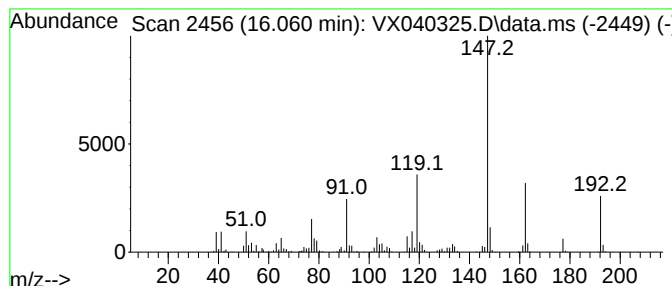
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Quant Title : SW846 8260

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

Peak Number 5 Ethanone, 1-(2,4,5-trimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.060	31.47 ug/l	535855	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(2,4,5-trimethylphen...	162	C11H14O	002040-07-5	95
2			Ethanone, 1-(2,3,4-trimethylphen...	162	C11H14O	001467-36-3	90
3			Ethanone, 1-(2,4,6-trimethylphen...	162	C11H14O	001667-01-2	90
4			Benzene, 1,4-bis(1-methylethyl)-	162	C12H18	000100-18-5	81
5			Benzene, 1,3-bis(1-methylethyl)-	162	C12H18	000099-62-7	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Octanone	11.835	10.8	ug/l	183566	4	12.024	851317	50.0
Naphthalene, 1,...	13.420	9.6	ug/l	162569	4	12.024	851317	50.0
Naphthalene, 2-...	15.207	27.6	ug/l	470811	4	12.024	851317	50.0
Diphenyl ether	15.323	65.2	ug/l	1109530	4	12.024	851317	50.0
Ethanone, 1-(2,...	16.060	31.5	ug/l	535855	4	12.024	851317	50.0