

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
 Data File : VX040326.D
 Acq On : 19 Feb 2024 13:30
 Operator : JC/MD
 Sample : P1395-04 40X
 Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 B-2(6-8)

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: VX040326.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	692	705	720	rBV	63597	184963	3.35%	1.567%
2	5.549	720	732	753	rVB	103762	301100	5.46%	2.551%
3	5.958	788	799	806	rBV	72676	194081	3.52%	1.644%
4	6.037	806	812	823	rVB2	25820	70822	1.28%	0.600%
5	6.763	920	931	945	rBV	168340	408981	7.41%	3.465%
6	7.122	979	990	1005	rBV	64267	143712	2.60%	1.218%
7	8.646	1234	1240	1246	rBV	360377	562828	10.20%	4.769%
8	8.720	1246	1252	1278	rVB	3563055	5519552	100.00%	46.768%
9	10.055	1465	1471	1473	rBV	383710	550485	9.97%	4.664%
10	10.073	1473	1474	1488	rVB	233467	270531	4.90%	2.292%
11	10.195	1488	1494	1504	rBV	85436	116983	2.12%	0.991%
12	10.299	1504	1511	1518	rBV	368877	500572	9.07%	4.241%
13	10.646	1562	1568	1580	rBV2	124433	229198	4.15%	1.942%
14	11.079	1634	1639	1651	rBV	314237	400996	7.27%	3.398%
15	12.024	1788	1794	1812	rVB3	411344	783402	14.19%	6.638%
16	12.335	1838	1845	1851	rBV	46828	62103	1.13%	0.526%
17	13.420	2019	2023	2026	rBV	62154	73864	1.34%	0.626%
18	13.774	2077	2081	2087	rBV	47293	58429	1.06%	0.495%
19	15.206	2310	2316	2326	rBV	217187	297860	5.40%	2.524%
20	15.322	2326	2335	2341	rBV	537982	706088	12.79%	5.983%
21	16.060	2448	2456	2464	rBV	230620	365418	6.62%	3.096%

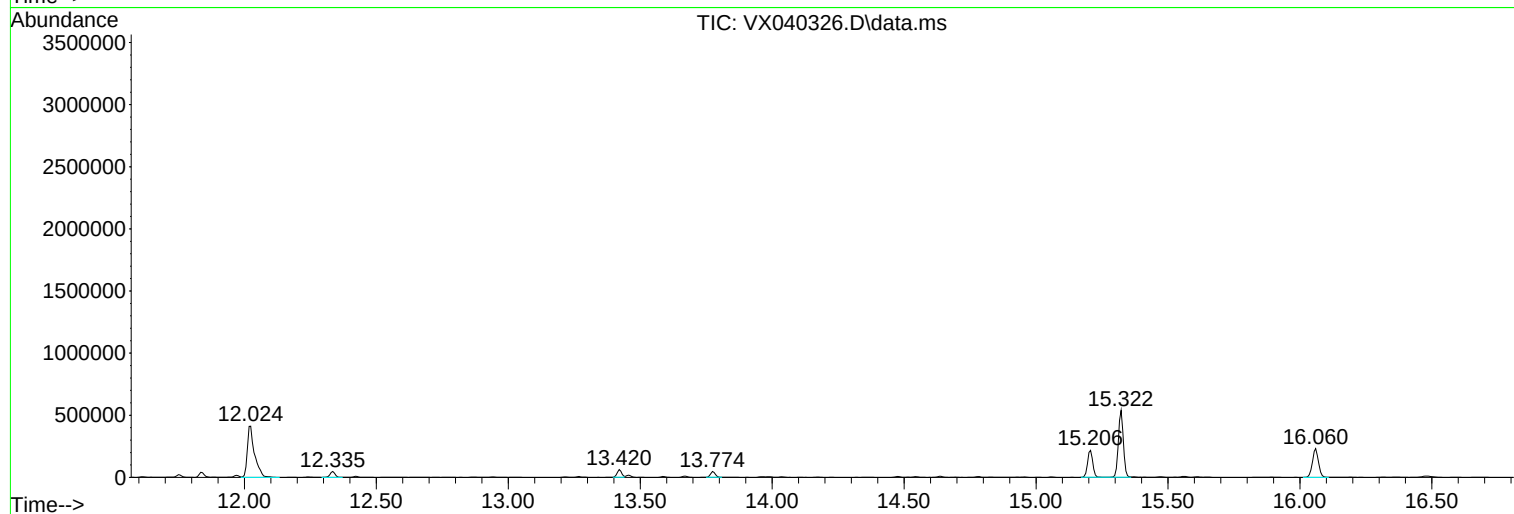
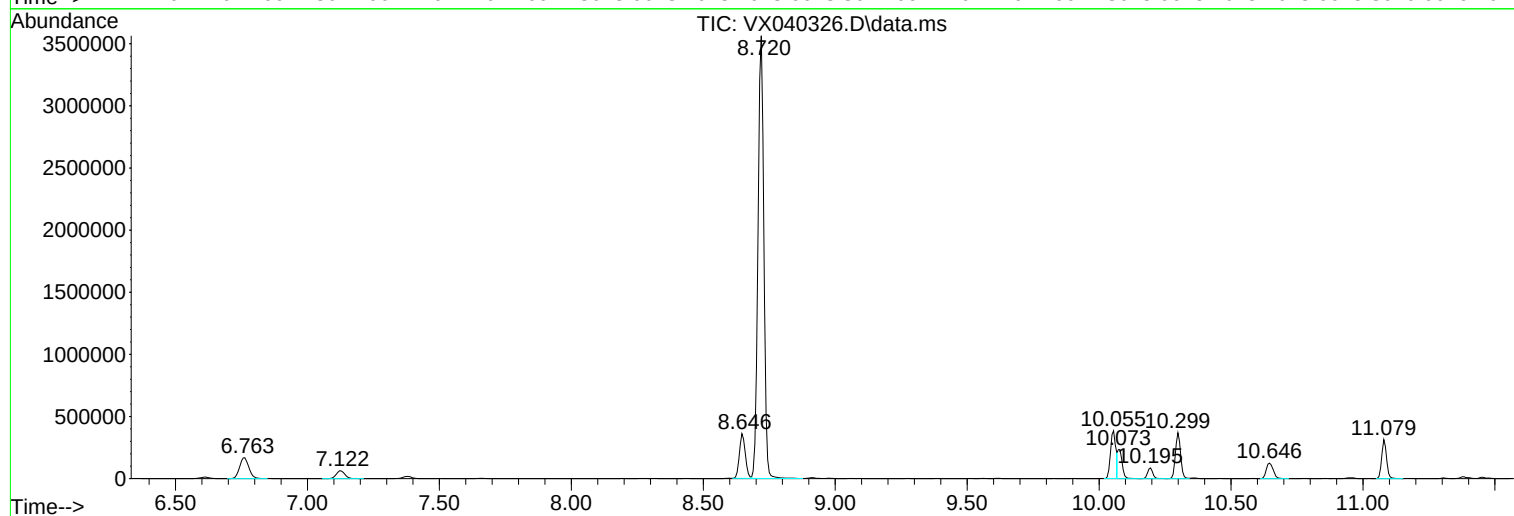
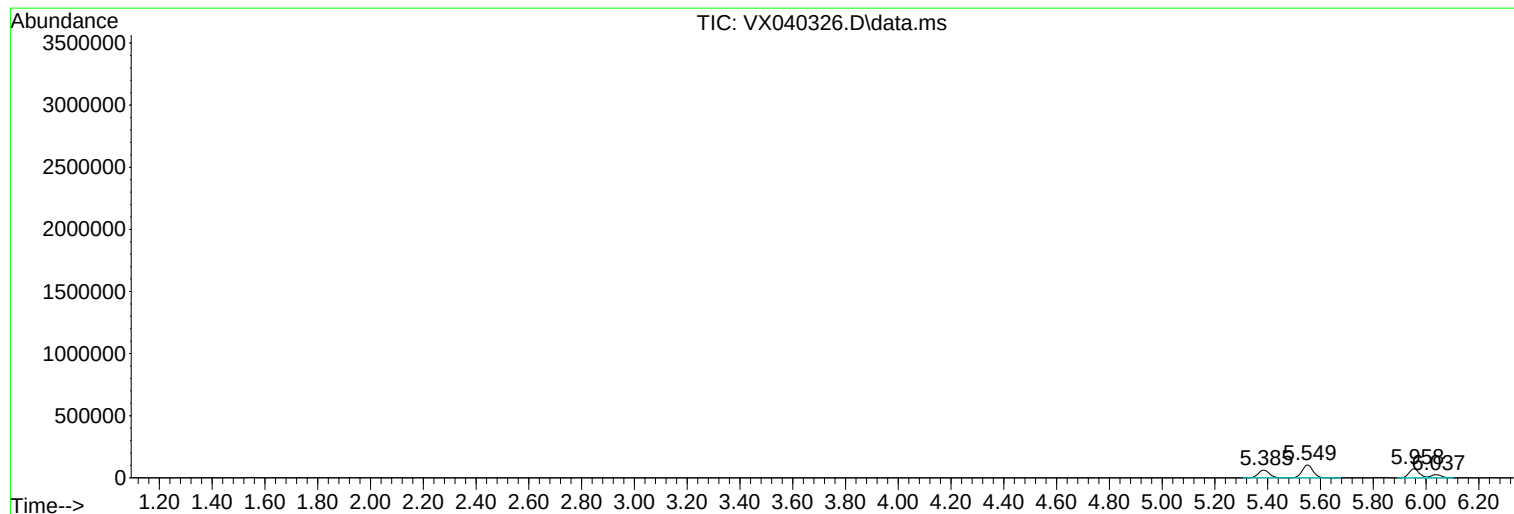
Sum of corrected areas: 11801968

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
Data File : VX040326.D
Acq On : 19 Feb 2024 13:30
Operator : JC/MD
Sample : P1395-04 40X
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-2(6-8)

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
Data File : VX040326.D
Acq On : 19 Feb 2024 13:30
Operator : JC/MD
Sample : P1395-04 40X
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-2(6-8)

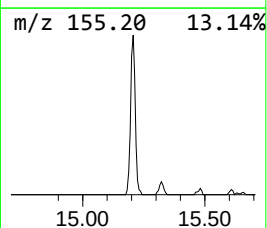
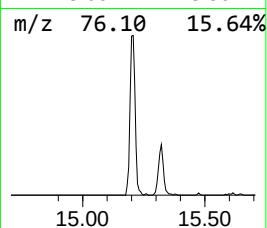
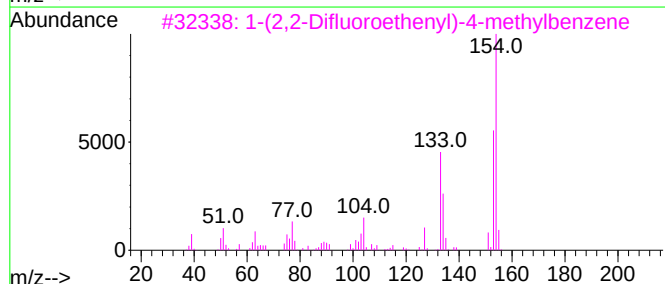
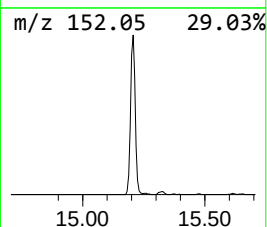
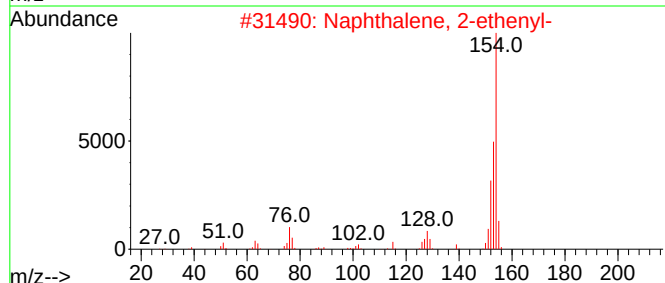
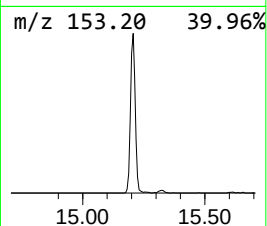
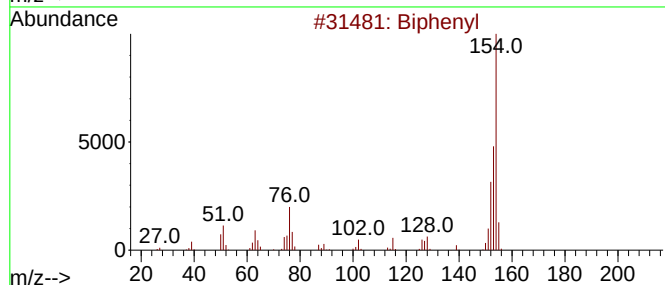
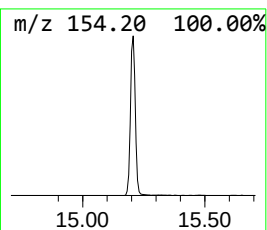
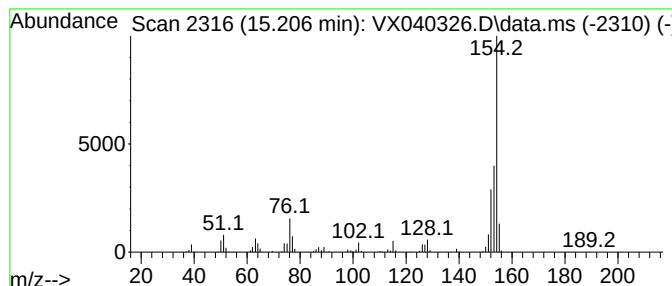
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, 2-ethenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.206	19.01 ug/l	297860	1,4-Dichlorobenzene-d4	12.024

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	87
3			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	53
4			Acenaphthene	154	C12H10	000083-32-9	49
5			6-Cyanoquinoline	154	C10H6N2	023395-72-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
Data File : VX040326.D
Acq On : 19 Feb 2024 13:30
Operator : JC/MD
Sample : P1395-04 40X
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-2(6-8)

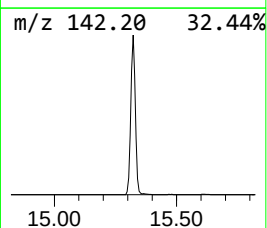
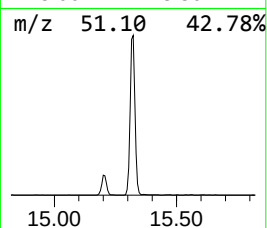
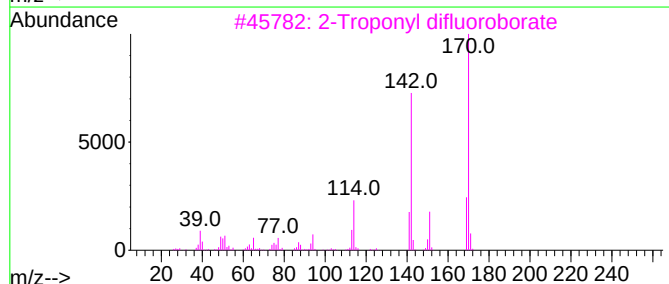
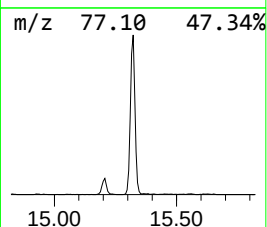
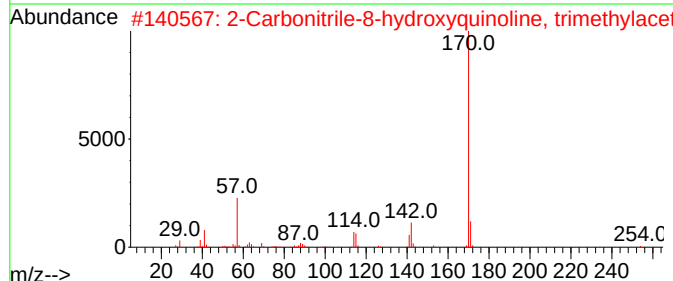
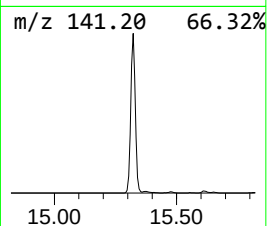
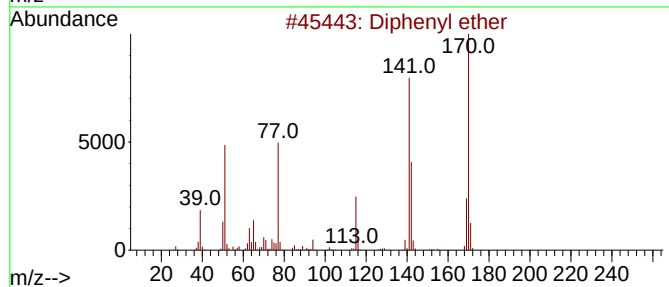
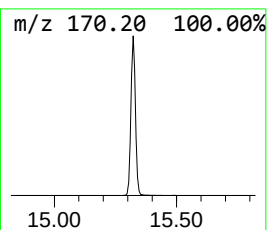
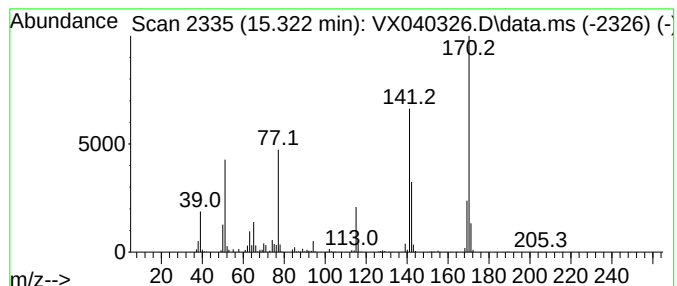
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 2 Diphenyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.322	45.07 ug/l	706088	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			2-Carbonitrile-8-hydroxyquinolin...	254	C15H14N2O2	1000463-12-5	38
3			2-Troponyl difluoroborate	170	C7H5BF2O2	022502-10-9	38
4			2-(2-Cyanophenyl)oxazole	170	C10H6N2O	1000281-31-2	38
5			Phenol, O-(ethylsulfinyl)-	170	C8H10O2S	029634-40-0	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
Data File : VX040326.D
Acq On : 19 Feb 2024 13:30
Operator : JC/MD
Sample : P1395-04 40X
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-2(6-8)

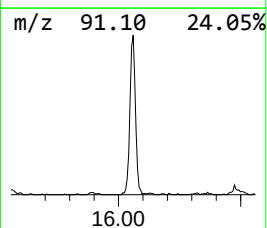
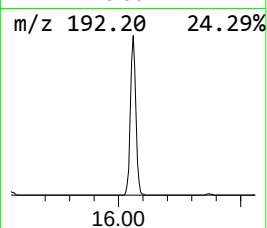
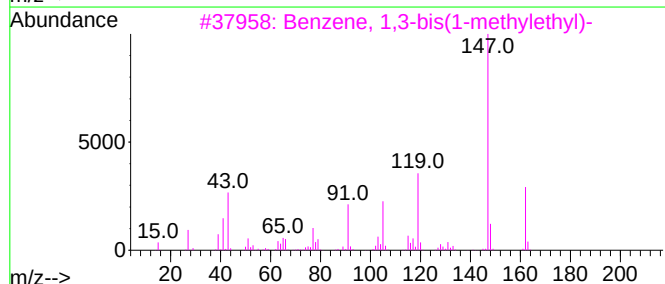
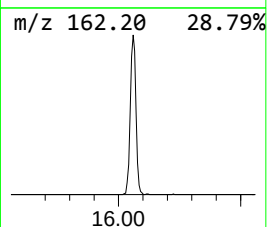
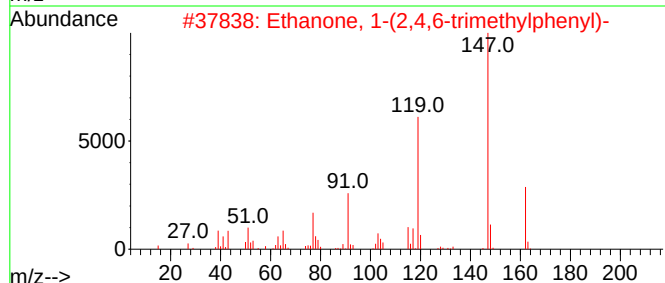
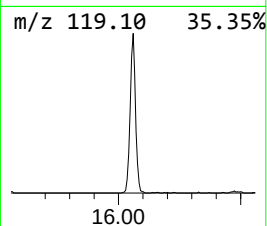
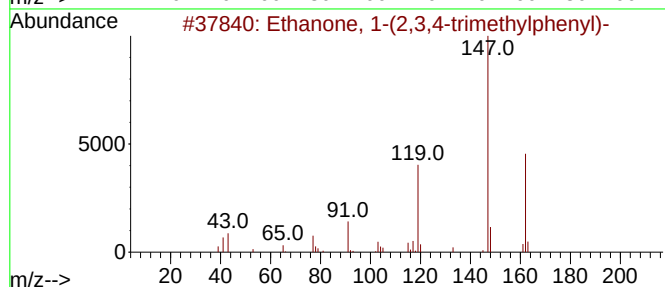
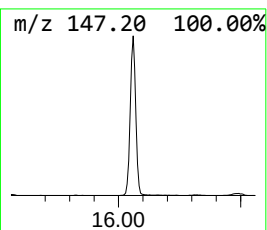
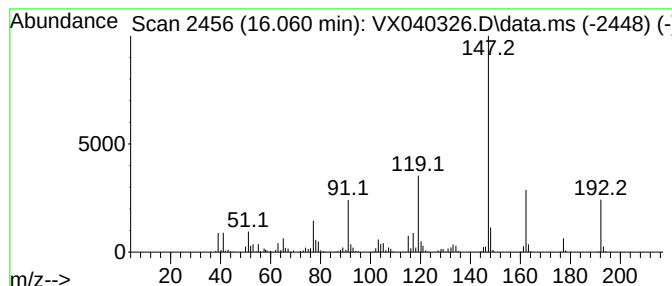
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethanone, 1-(2,3,4-trimethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.060	23.32 ug/l	365418	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(2,3,4-trimethylphen...	162	C11H14O	001467-36-3	93
2			Ethanone, 1-(2,4,6-trimethylphen...	162	C11H14O	001667-01-2	90
3			Benzene, 1,3-bis(1-methylethyl)-	162	C12H18	000099-62-7	87
4			Benzene, 1,4-bis(1-methylethyl)-	162	C12H18	000100-18-5	81
5			4-(t-Butyl)benzaldehyde	162	C11H14O	000939-97-9	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021924\
Data File : VX040326.D
Acq On : 19 Feb 2024 13:30
Operator : JC/MD
Sample : P1395-04 40X
Misc : 3.42g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
B-2(6-8)

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 2-...	15.206	19.0	ug/l	297860	4	12.024	783402	50.0
Diphenyl ether	15.322	45.1	ug/l	706088	4	12.024	783402	50.0
Ethanone, 1-(2,...	16.060	23.3	ug/l	365418	4	12.024	783402	50.0