

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
 Data File : VX045832.D
 Acq On : 17 Apr 2025 16:42
 Operator : JC/MD
 Sample : Q1818-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 3651

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\82X040225W.M
 Title : SW846 8260

Signal : TIC: VX045832.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	38	44	50	rBV	12514	14630	2.98%	0.489%
2	1.617	70	87	90	rBV6	5926	23720	4.83%	0.793%
3	2.380	207	212	216	rBV	7300	12332	2.51%	0.412%
4	2.550	234	240	247	rVB2	3936	7895	1.61%	0.264%
5	2.971	298	309	321	rBV	11512	29185	5.94%	0.976%
6	5.379	692	704	721	rBV	55891	167116	34.04%	5.588%
7	5.544	721	731	746	rVV2	81445	235878	48.04%	7.888%
8	5.952	789	798	812	rBV2	66297	177459	36.14%	5.934%
9	6.757	921	930	944	rBV	143779	351788	71.65%	11.764%
10	8.647	1233	1240	1260	rVV	305512	491009	100.00%	16.420%
11	10.049	1465	1470	1487	rBV	311074	440685	89.75%	14.737%
12	11.079	1630	1639	1650	rBV	262465	339401	69.12%	11.350%
13	12.018	1788	1793	1803	rBV	315450	391961	79.83%	13.107%
14	12.201	1819	1823	1830	rVB4	3791	6678	1.36%	0.223%
15	12.823	1919	1925	1938	rBV	39918	60682	12.36%	2.029%
16	14.225	2149	2155	2159	rVV8	4621	10174	2.07%	0.340%
17	14.475	2192	2196	2201	rBV7	5167	11493	2.34%	0.384%
18	14.615	2215	2219	2220	rBV3	10065	10561	2.15%	0.353%
19	14.755	2239	2242	2244	rBV4	4822	6141	1.25%	0.205%
20	15.560	2371	2374	2378	rVB3	14508	19773	4.03%	0.661%
21	15.993	2442	2445	2455	rVB5	26003	50915	10.37%	1.703%
22	16.090	2455	2461	2468	rBV	72112	130903	26.66%	4.377%

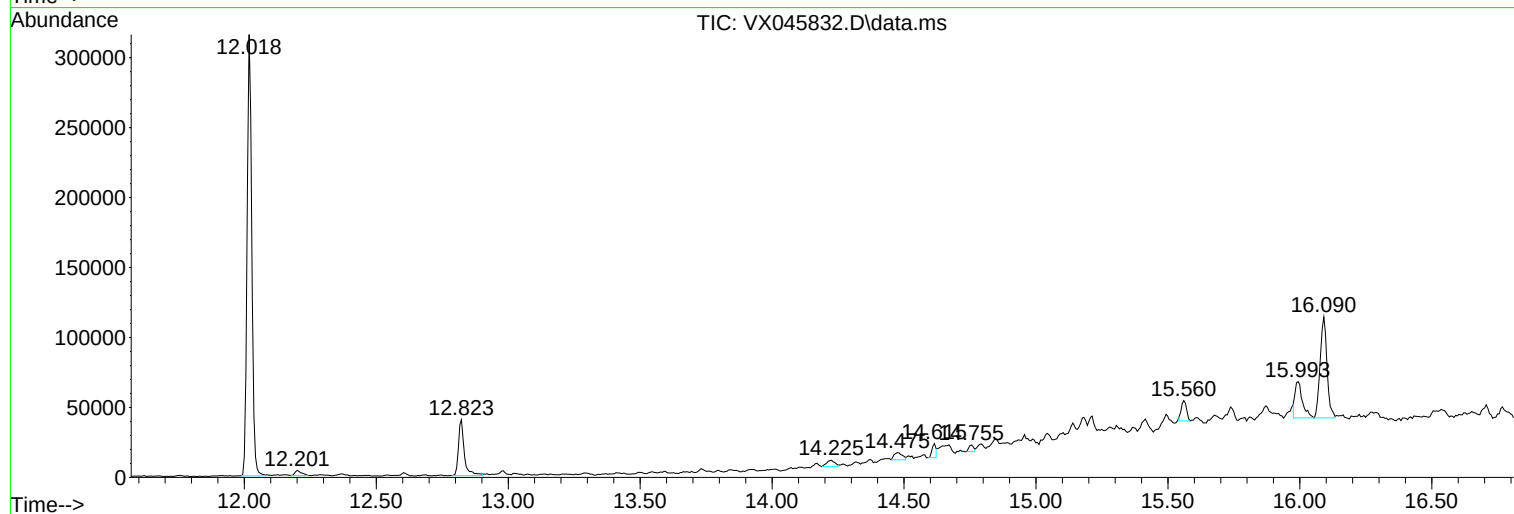
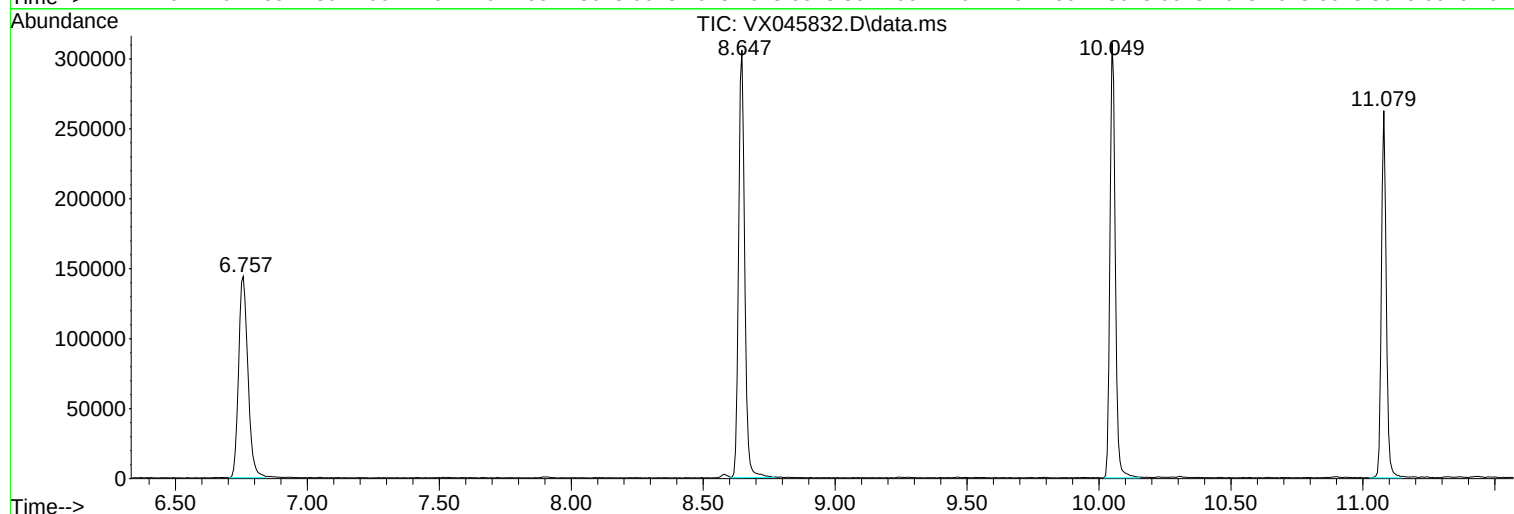
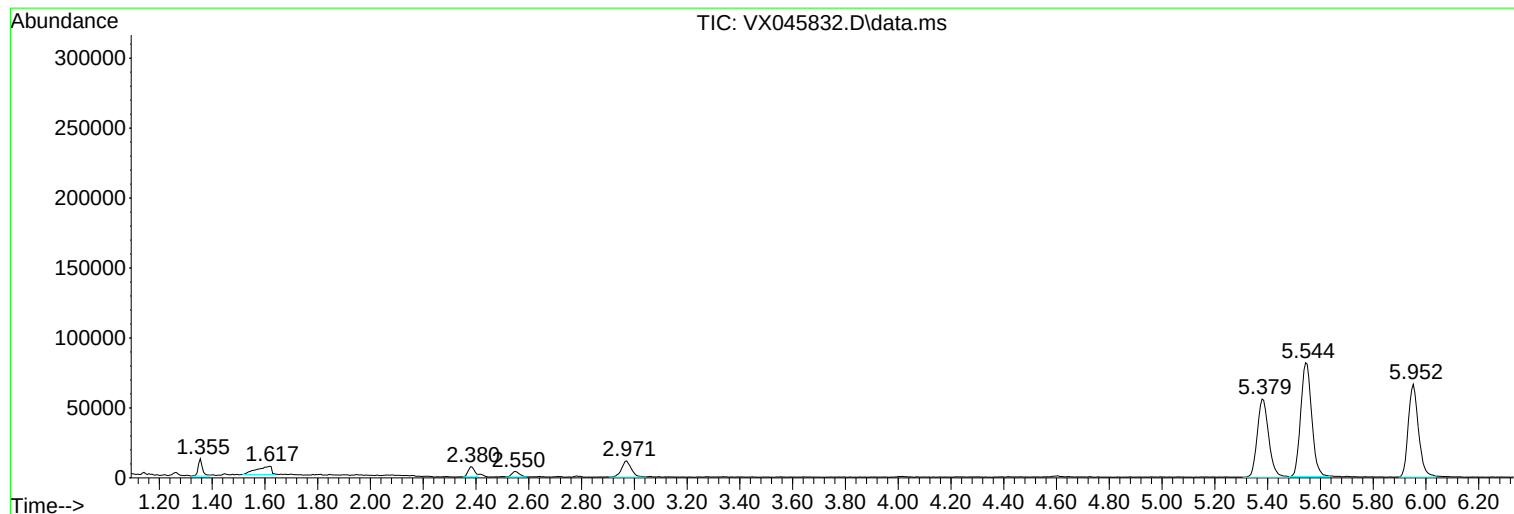
Sum of corrected areas: 2990379

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045832.D
Acq On : 17 Apr 2025 16:42
Operator : JC/MD
Sample : Q1818-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3651

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045832.D
Acq On : 17 Apr 2025 16:42
Operator : JC/MD
Sample : Q1818-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3651

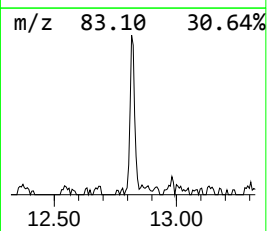
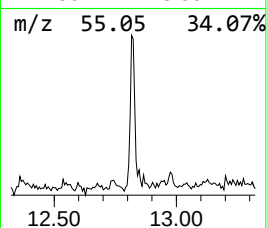
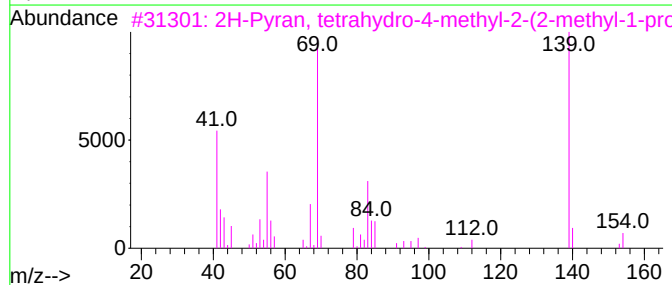
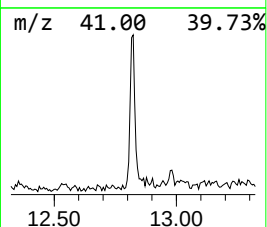
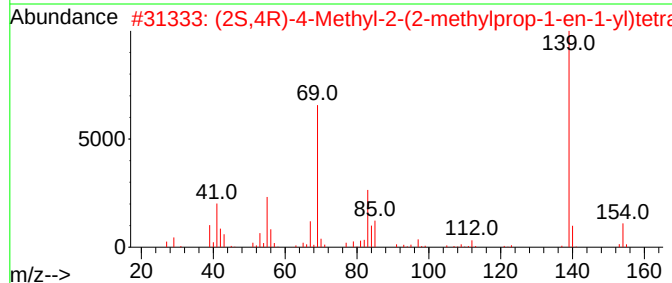
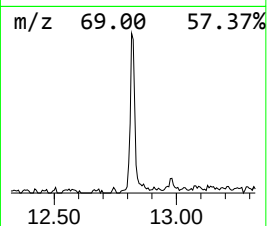
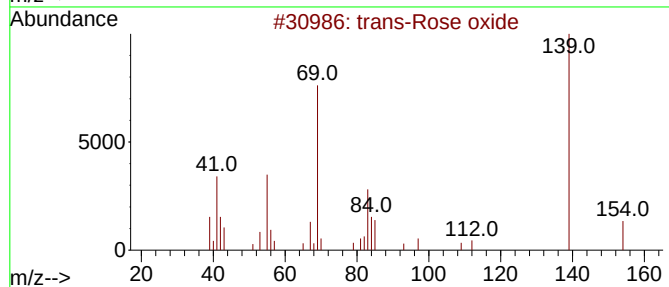
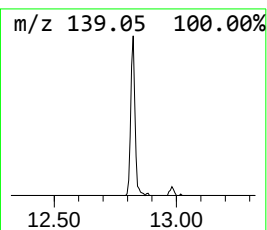
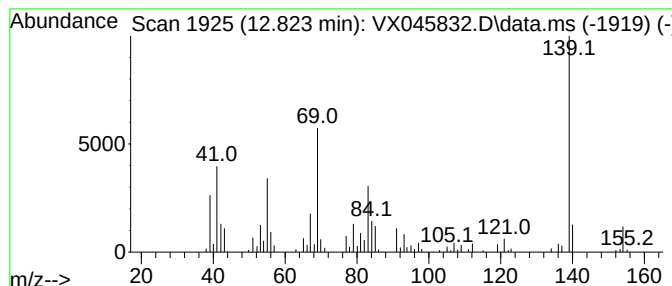
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 2 trans-Rose oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.823	7.74 ug/l	60682	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Rose oxide	154	C10H18O	000876-18-6	96
2			(2S,4R)-4-Methyl-2-(2-methylprop...	154	C10H18O	003033-23-6	93
3			2H-Pyran, tetrahydro-4-methyl-2-...	154	C10H18O	016409-43-1	90
4			(2R,4R)-4-Methyl-2-(2-methylprop...	154	C10H18O	005258-11-7	90
5			3-Pyridinecarboxylic acid, 6-hyd...	139	C6H5NO3	005006-66-6	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045832.D
Acq On : 17 Apr 2025 16:42
Operator : JC/MD
Sample : Q1818-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3651

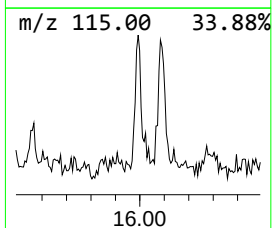
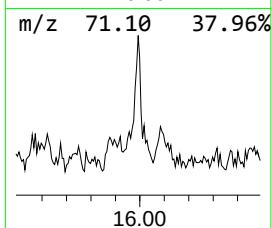
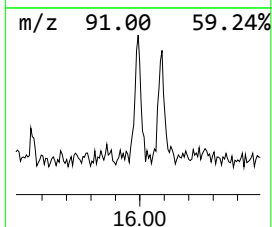
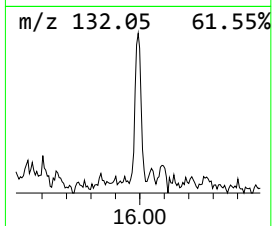
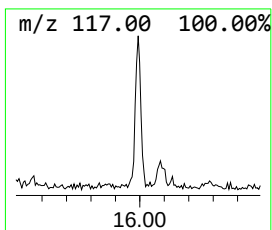
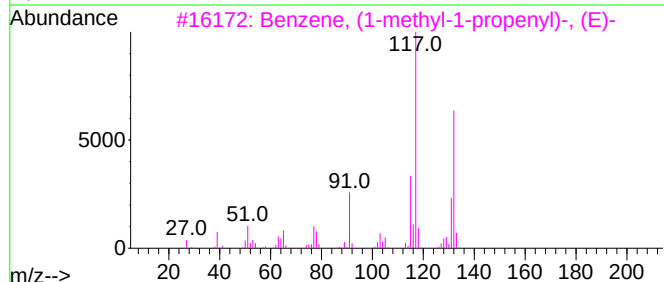
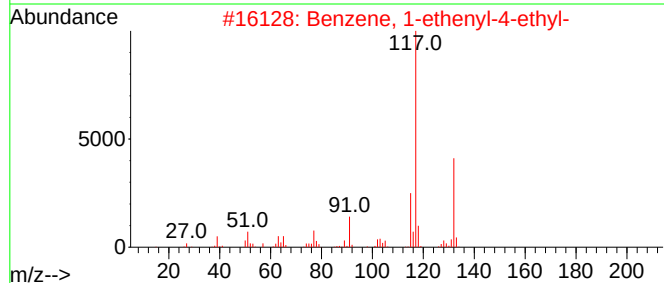
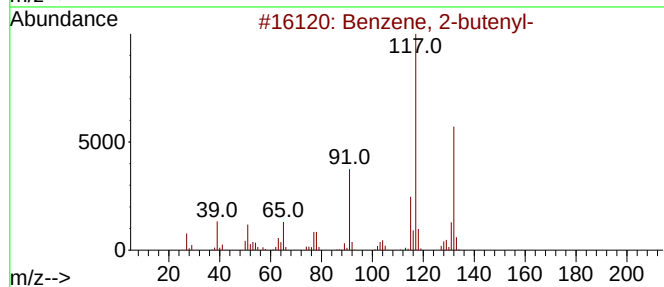
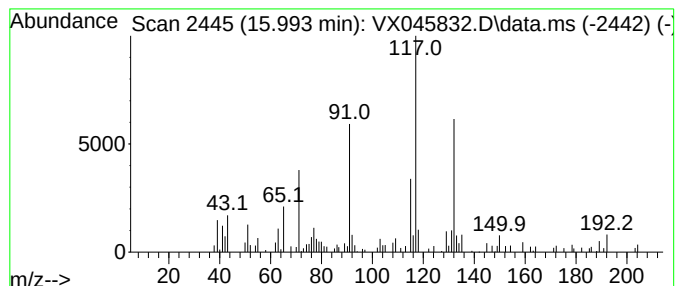
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 2-butenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.993	6.49 ug/l	50915	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-butenyl-	132	C10H12	001560-06-1	76
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	70
3			Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	70
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045832.D
Acq On : 17 Apr 2025 16:42
Operator : JC/MD
Sample : Q1818-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3651

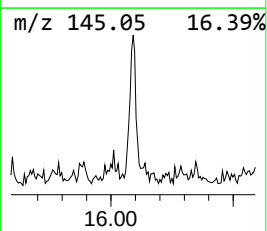
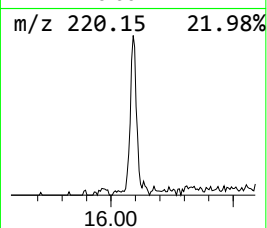
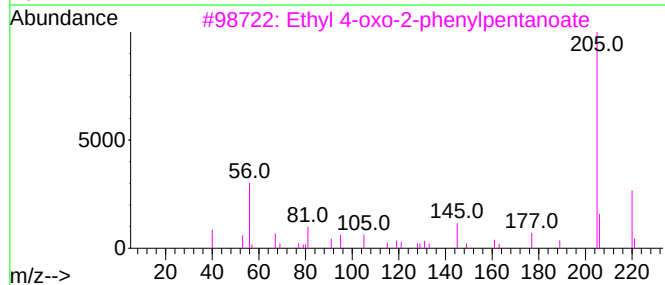
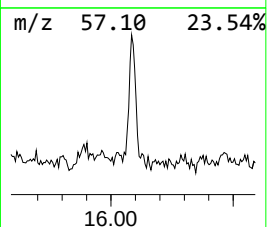
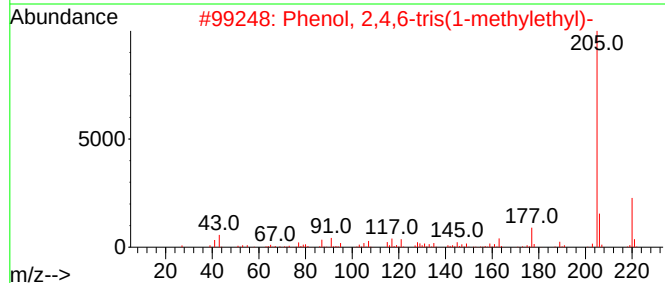
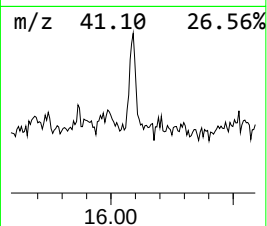
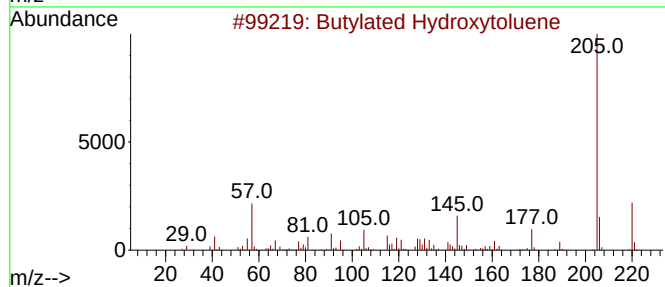
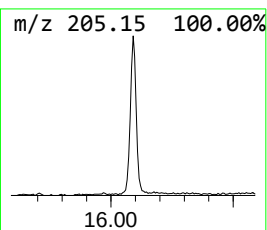
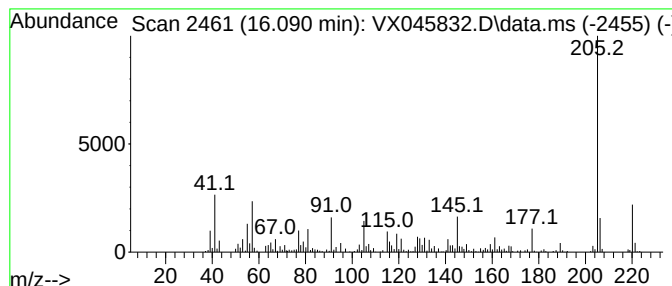
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.M
Quant Title : SW846 8260

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.090	16.70 ug/l	130903	1,4-Dichlorobenzene-d4	12.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	90
3			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	90
4			Phenol, 4,6-di(1,1-dimethylethyl)-	220	C15H24O	000616-55-7	81
5			4,6-di-tert-Butyl-m-cresol	220	C15H24O	000497-39-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041725\
Data File : VX045832.D
Acq On : 17 Apr 2025 16:42
Operator : JC/MD
Sample : Q1818-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
3651

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X040225W.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
trans-Rose oxide	12.823	7.7	ug/l	60682	4	12.018	391961	50.0
Benzene, 2-bute...	15.993	6.5	ug/l	50915	4	12.018	391961	50.0
Butylated Hydro...	16.090	16.7	ug/l	130903	4	12.018	391961	50.0