

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
 Data File : VX043375.D
 Acq On : 14 Oct 2024 12:12
 Operator : JC/MD
 Sample : P4394-01 20X
 Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WASH-DEBRIS

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\82X100124W.M
 Title : SW846 8260

Signal : TIC: VX043375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.557	69	77	79	rBV4	3799	8169	1.45%	0.159%
2	1.642	81	91	92	rVV6	2430	7579	1.34%	0.148%
3	2.947	298	305	316	rBV	5703	13558	2.40%	0.265%
4	5.385	693	705	722	rBV	54126	161204	28.59%	3.145%
5	5.550	722	732	750	rVB	88003	256840	45.55%	5.011%
6	5.952	789	798	816	rBV2	64750	173917	30.84%	3.393%
7	6.757	920	930	950	rBV	146316	354602	62.88%	6.919%
8	8.647	1233	1240	1255	rBV	293079	470439	83.42%	9.179%
9	10.049	1465	1470	1487	rBV	273027	403167	71.49%	7.867%
10	11.079	1634	1639	1650	rBV	230048	309471	54.88%	6.038%
11	11.616	1723	1727	1732	rBV7	3864	7179	1.27%	0.140%
12	11.756	1746	1750	1755	rVB	6291	9851	1.75%	0.192%
13	12.018	1789	1793	1800	rBV	273510	359594	63.77%	7.016%
14	12.311	1838	1841	1848	rBV6	9650	15829	2.81%	0.309%
15	12.817	1920	1924	1930	rVB4	23165	34970	6.20%	0.682%
16	12.981	1948	1951	1956	rVB4	13799	17676	3.13%	0.345%
17	13.036	1958	1960	1964	rVB5	10006	11988	2.13%	0.234%
18	13.292	1998	2002	2007	rVB4	30797	43285	7.68%	0.845%
19	13.414	2016	2022	2029	rBV5	37491	92385	16.38%	1.803%
20	13.500	2033	2036	2041	rVB6	11043	16692	2.96%	0.326%
21	13.585	2047	2050	2054	rBV5	13432	23376	4.15%	0.456%
22	13.676	2061	2065	2068	rBV5	13891	23066	4.09%	0.450%
23	13.737	2072	2075	2076	rBV2	8626	9627	1.71%	0.188%
24	13.798	2082	2085	2088	rBV3	24112	29374	5.21%	0.573%
25	13.847	2089	2093	2100	rVV5	27628	53003	9.40%	1.034%
26	13.920	2101	2105	2111	rVB9	17877	32565	5.77%	0.635%
27	14.061	2125	2128	2132	rBV4	20555	30448	5.40%	0.594%
28	14.225	2150	2155	2159	rBV5	38141	71093	12.61%	1.387%
29	14.481	2193	2197	2204	rBV6	38555	76797	13.62%	1.498%
30	14.554	2206	2209	2210	rBV3	12727	15018	2.66%	0.293%
31	14.615	2215	2219	2225	rVV	117341	174665	30.97%	3.408%
32	14.670	2225	2228	2232	rVV2	76025	84997	15.07%	1.658%
33	14.756	2239	2242	2244	rBV4	24779	26706	4.74%	0.521%
34	14.792	2245	2248	2250	rBV4	24955	31428	5.57%	0.613%
35	14.823	2250	2253	2254	rVV3	33245	37142	6.59%	0.725%
36	14.847	2254	2257	2261	rVB2	75442	94352	16.73%	1.841%

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

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37	14.920	2266	2269	2273	rBV4	27575	48877	8.67%	0.954%
38	15.042	2285	2289	2293	rVB3	32753	53668	9.52%	1.047%
39	15.182	2307	2312	2314	rBV3	83280	125848	22.32%	2.456%
40	15.243	2320	2322	2326	rVB2	32623	40548	7.19%	0.791%
41	15.377	2340	2344	2347	rBV4	38730	58519	10.38%	1.142%
42	15.414	2347	2350	2354	rVB2	63112	84773	15.03%	1.654%
43	15.487	2358	2362	2363	rBV3	44547	60774	10.78%	1.186%
44	15.853	2418	2422	2429	rBV8	46327	128206	22.74%	2.502%
45	16.091	2456	2461	2472	rBV	307201	563914	100.00%	11.003%
46	16.274	2487	2491	2502	rVB4	85004	274015	48.59%	5.347%
47	16.420	2511	2515	2525	rBV3	35526	103867	18.42%	2.027%

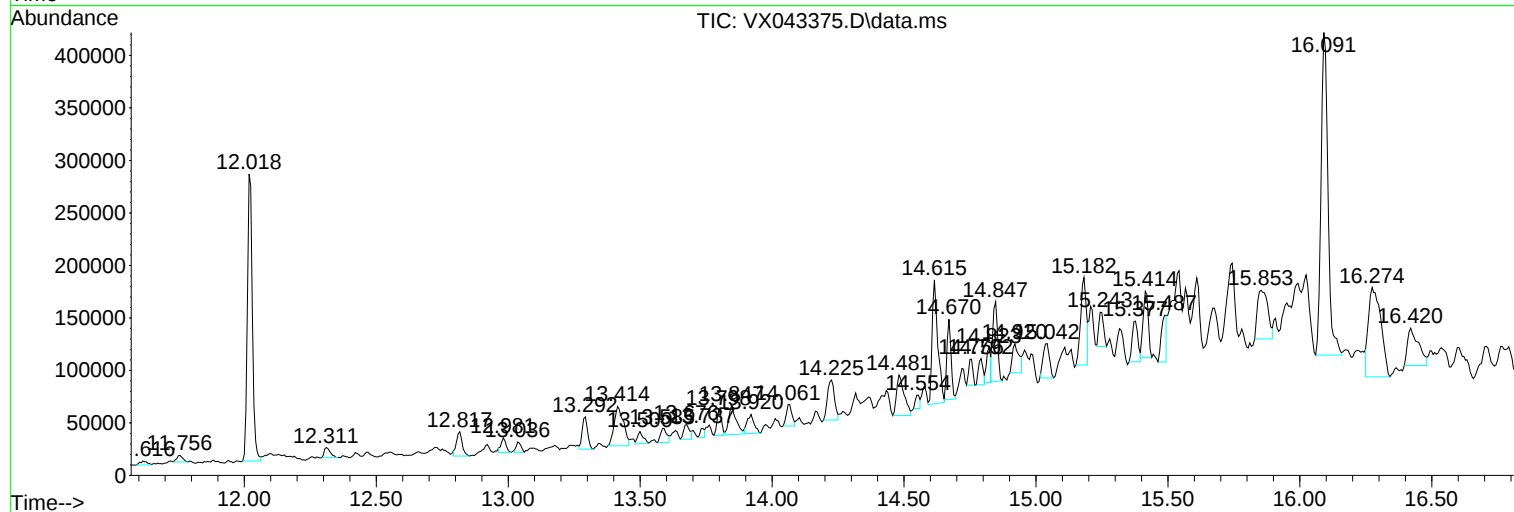
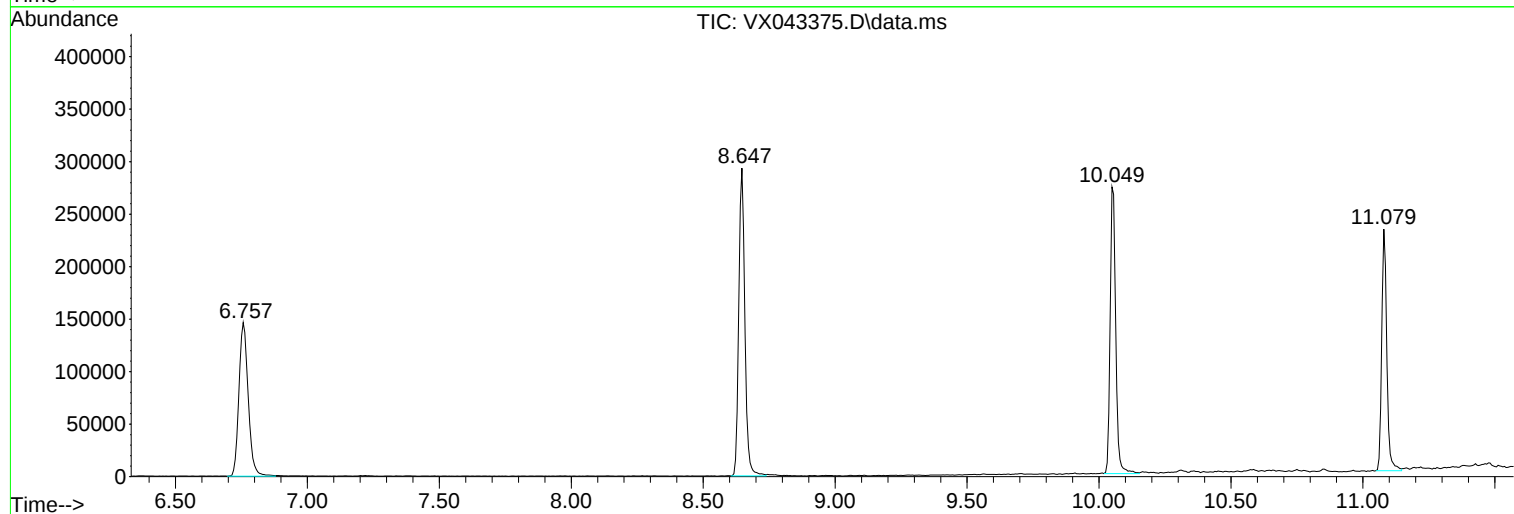
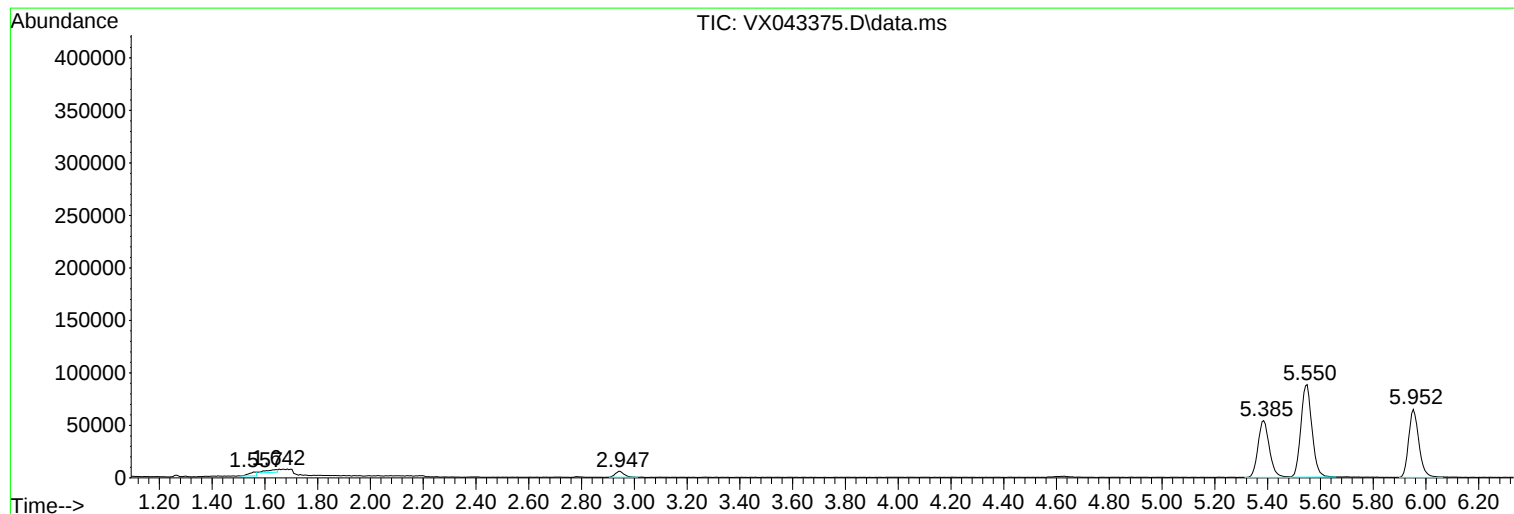
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Quant Title : SW846 8260

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



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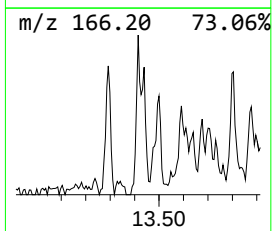
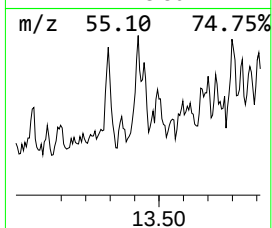
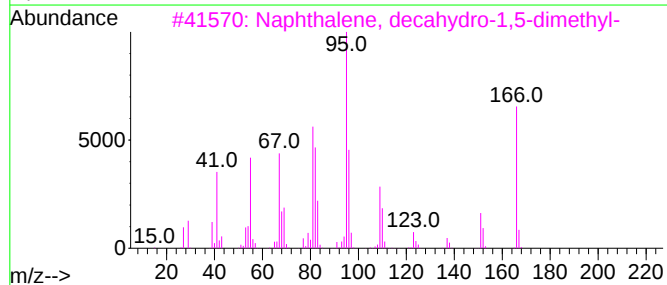
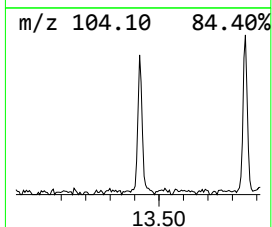
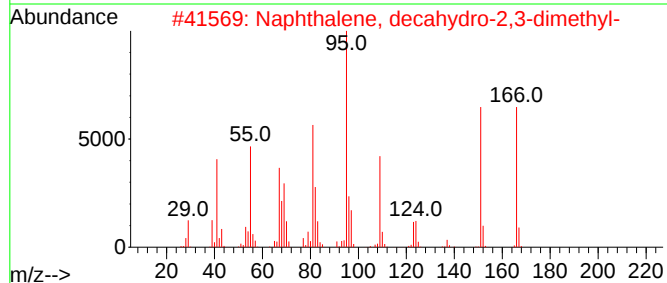
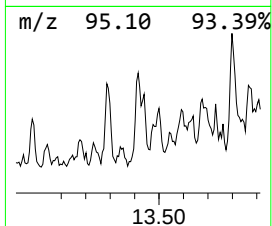
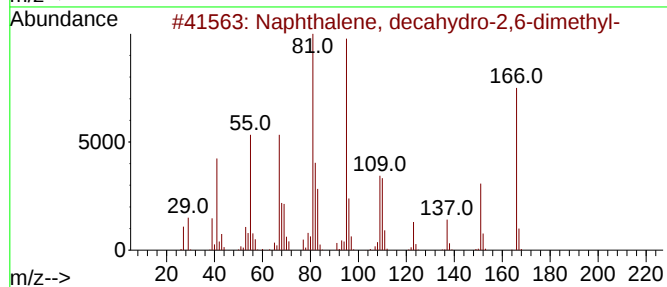
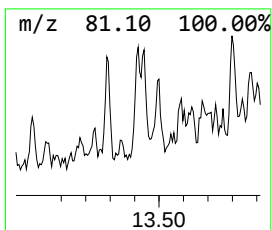
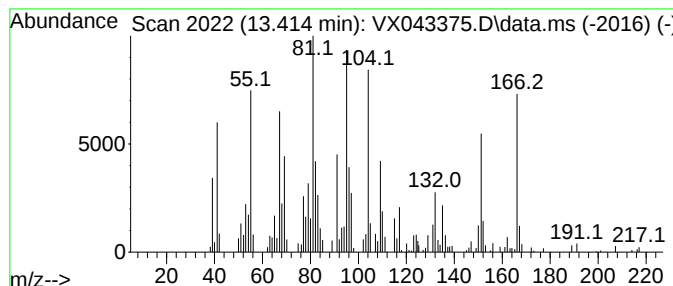
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 1 Naphthalene, decahydro-2,6-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	12.85 ug/l	92385	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	60
2			Naphthalene, decahydro-2,3-dimet...	166	C12H22	001008-80-6	46
3			Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	42
4			Cyclodecene, 1-methyl-	152	C11H20	066633-38-3	38
5			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	38



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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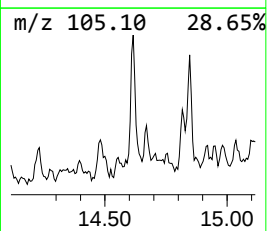
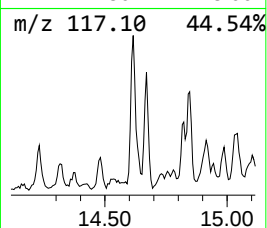
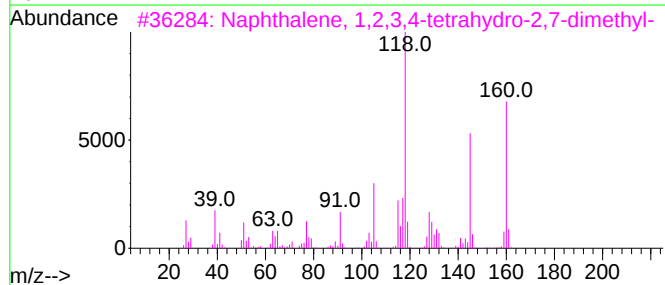
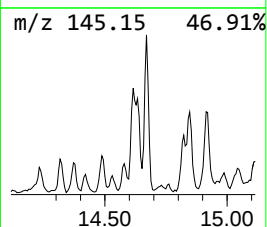
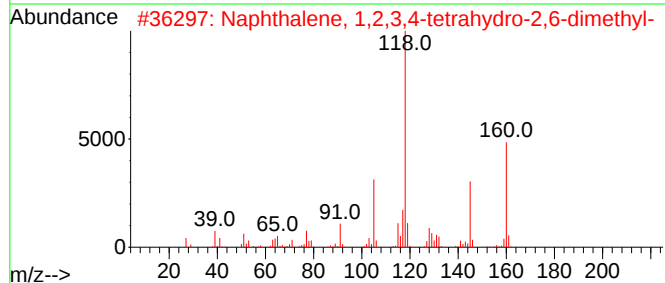
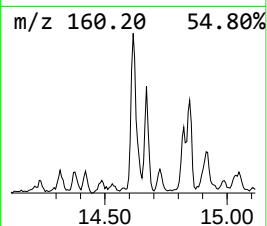
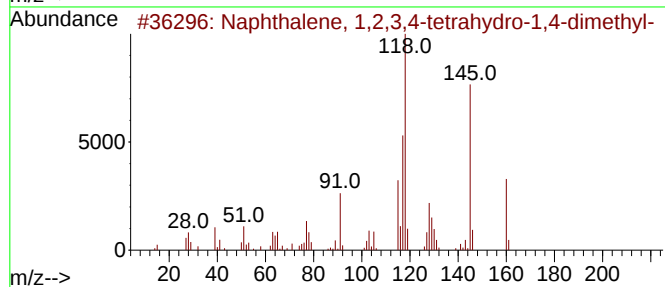
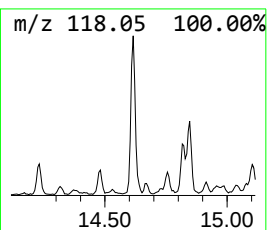
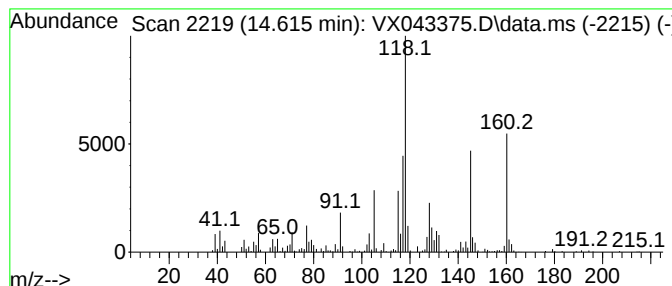
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.615	24.29 ug/l	174665	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	007524-63-2	81
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	013065-07-1	81
4			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	014944-23-1	64
5			Benzene, (3-methyl-1-methylenebu...	160	C12H16	038212-14-5	58



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Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

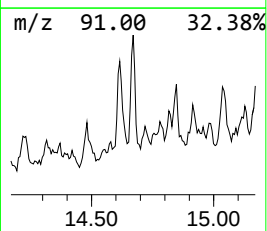
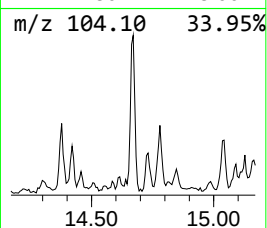
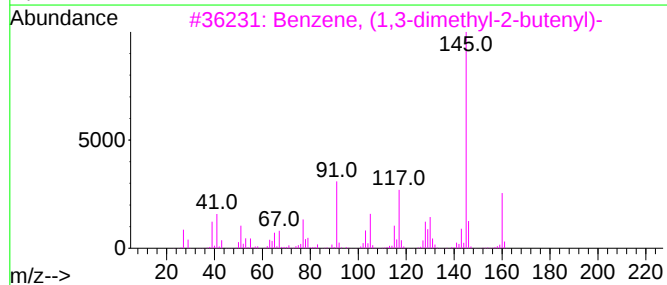
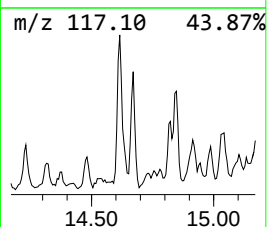
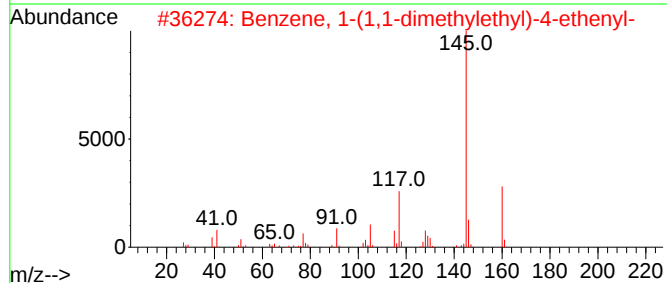
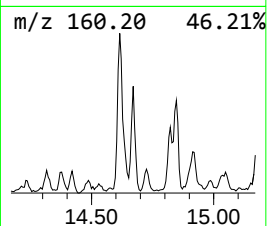
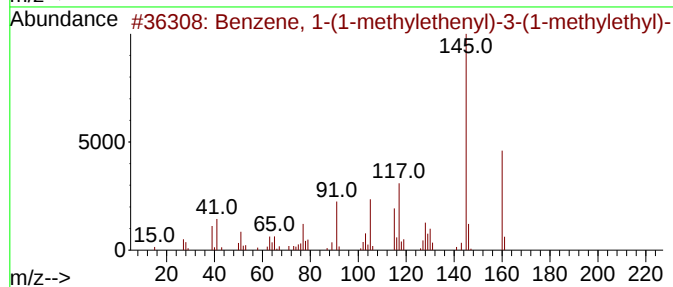
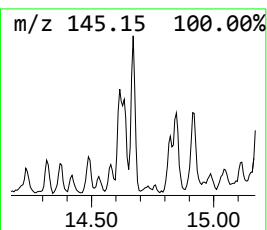
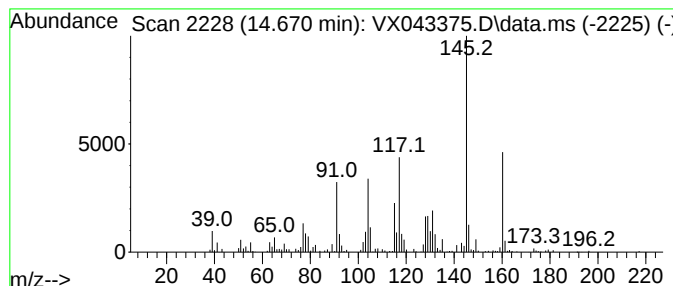
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-(1-methylethenyl)... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.670	11.82 ug/l	84997	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	81
2			Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	76
3			Benzene, (1,3-dimethyl-2-butenyl)-	160	C12H16	050704-01-3	74
4			1H-Indene, 2,3-dihydro-1,1,5-tri...	160	C12H16	040650-41-7	70
5			Benzene, 1-(1-methylethenyl)-2-(...	160	C12H16	005557-93-7	68



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Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

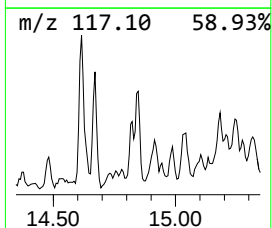
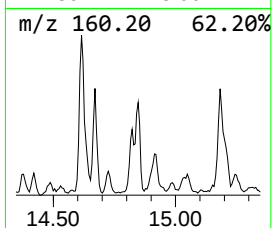
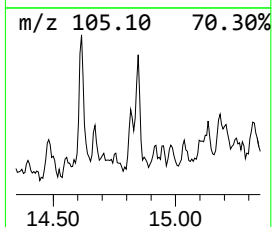
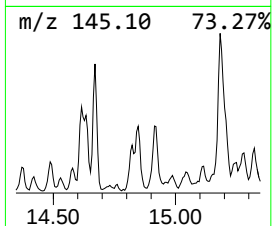
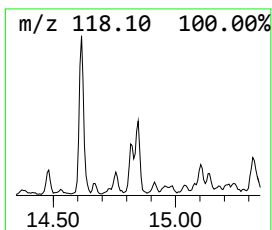
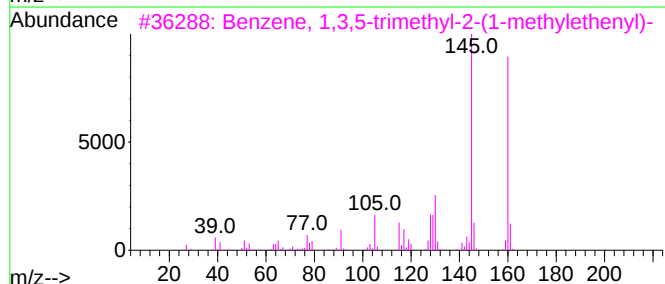
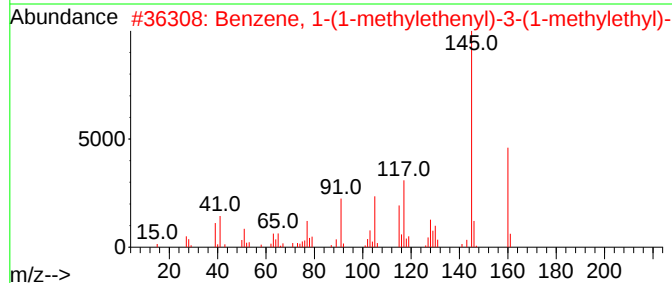
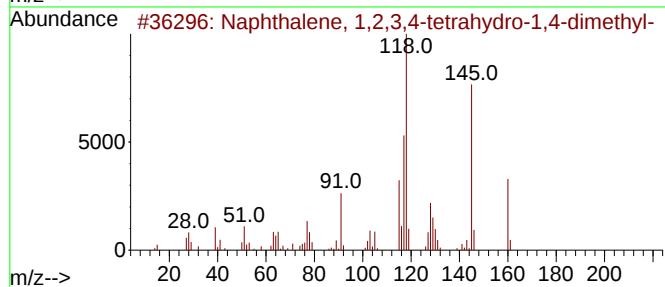
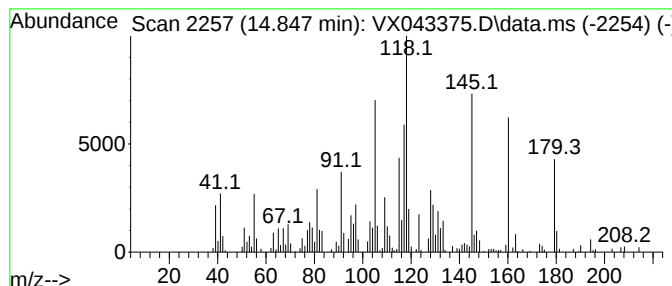
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Quant Title : SW846 8260

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

Peak Number 4 unknown14.847 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	13.12 ug/l	94352	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	76
2			Benzene, 1-(1-methylethenyl)-3-(...	160	C12H16	001129-29-9	55
3			Benzene, 1,3,5-trimethyl-2-(1-me...	160	C12H16	014679-13-1	46
4			Benzene, 1-(1,1-dimethylethyl)-4...	160	C12H16	001746-23-2	41
5			2-Chloro-6-fluorophenol, methyl ...	160	C7H6ClFO	1000352-53-9	38



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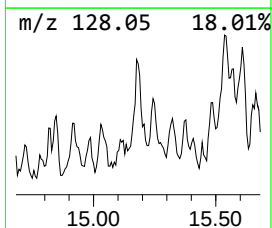
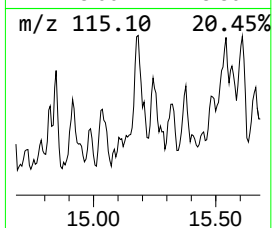
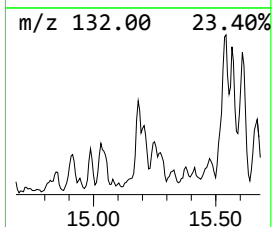
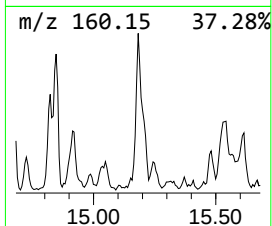
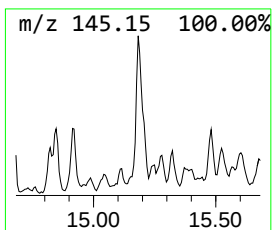
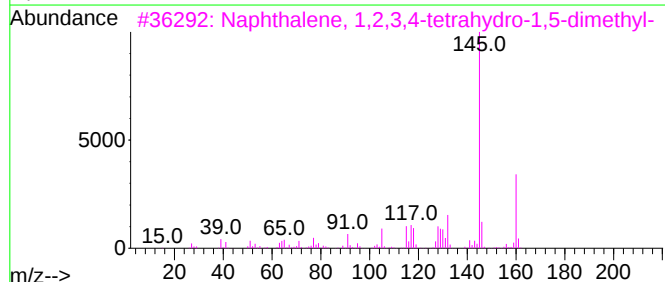
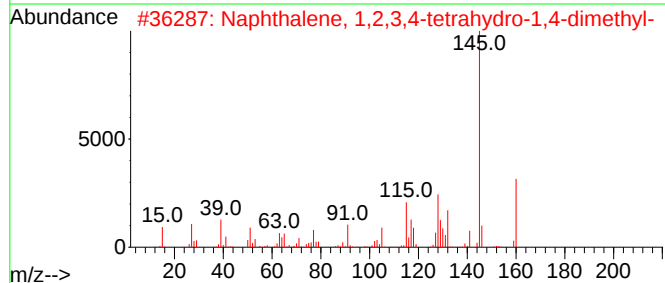
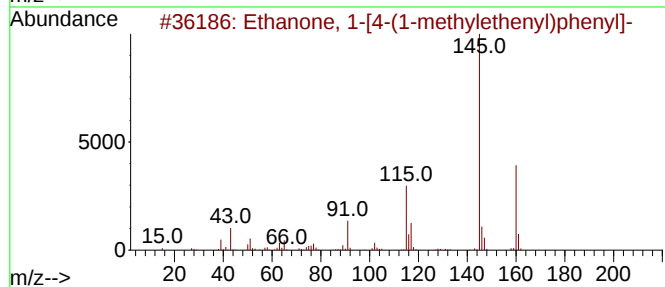
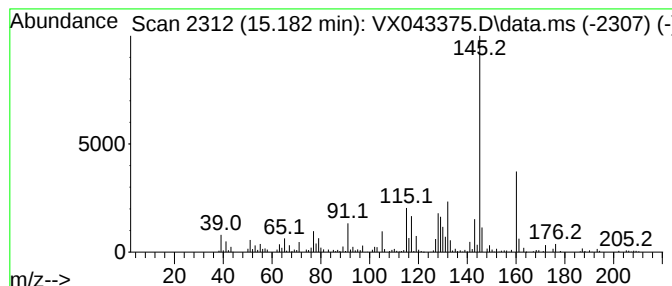
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Quant Title : SW846 8260

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

Peak Number 5 Ethanone, 1-[4-(1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.182	17.50 ug/l	125848	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-[4-(1-methylethenyl)...	160	C11H12O	005359-04-6	93
2			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	93
3			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	021564-91-0	91
4			1H-Indene, 2,3-dihydro-1,1,3-tri...	160	C12H16	002613-76-5	87
5			1H-Inden-1-one, 2,3-dihydro-3,3-...	160	C11H12O	026465-81-6	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

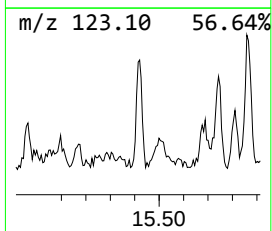
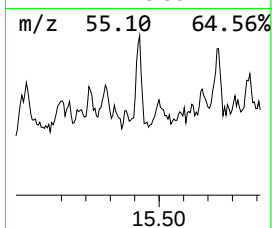
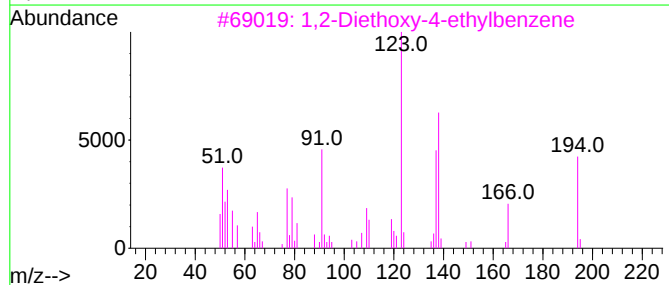
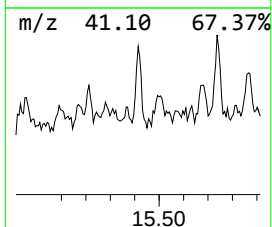
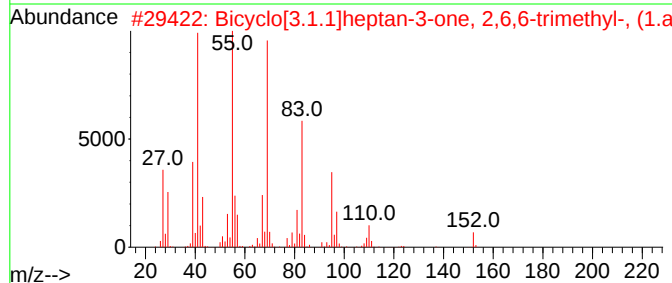
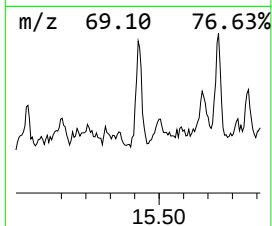
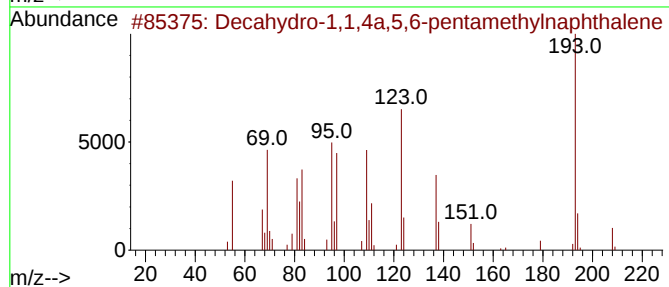
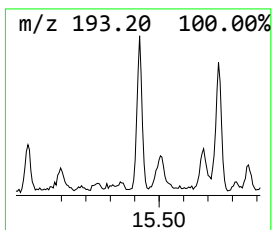
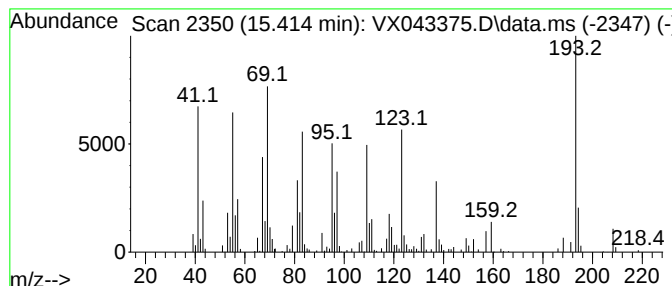
Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 6 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
15.414	11.79 ug/l	84773	1,4-Dichlorobenzene-d4			12.024
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	83
2	Bicyclo[3.1.1]heptan-3-one, 2,6,...		152	C10H16O	015358-88-0	30
3	1,2-Diethoxy-4-ethylbenzene		194	C12H18O2	131358-04-8	25
4	3,5-Diamino-6-[2-thienyl]-1,2,4-...		193	C7H7N5S	058848-66-1	22
5	1-(p-Fluorophenyl)-4-piperidone		193	C11H12FNO	1000238-56-7	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

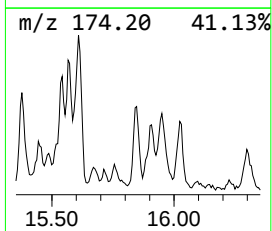
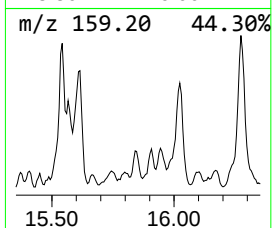
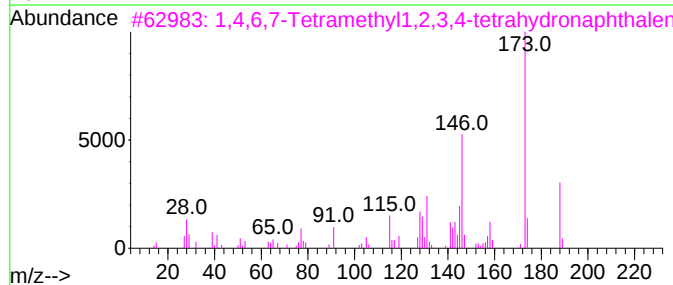
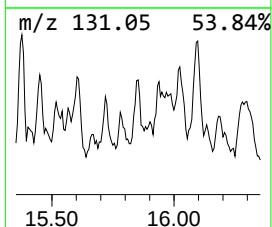
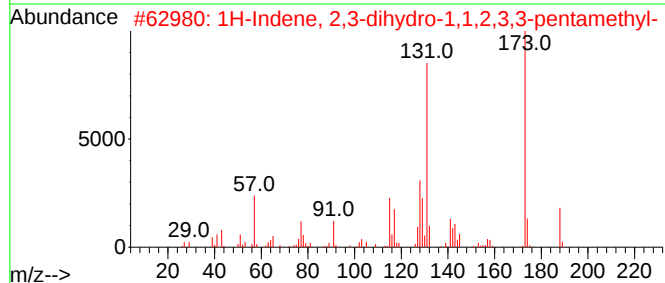
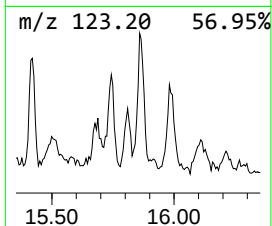
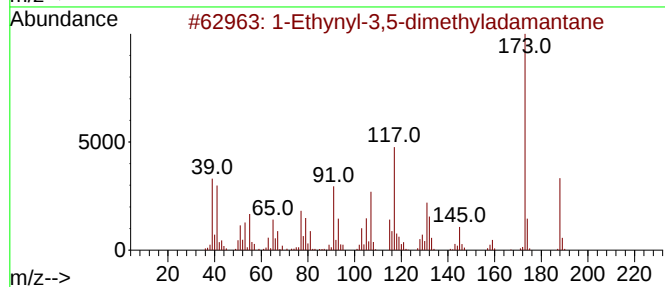
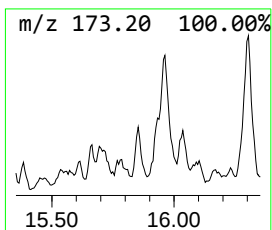
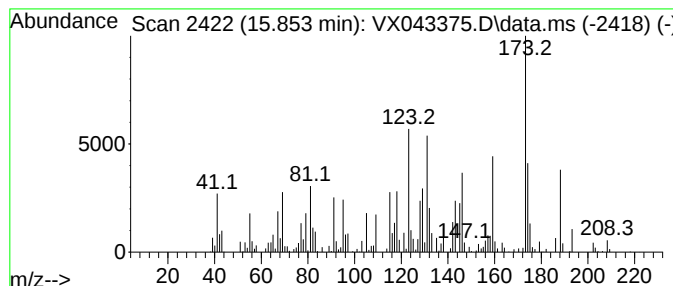
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Quant Title : SW846 8260

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

Peak Number 7 unknown15.853 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.853	17.83 ug/l	128206	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethynyl-3,5-dimethyladamantane	188	C14H20	1000245-73-3	38
2			1H-Indene, 2,3-dihydro-1,1,2,3,3...	188	C14H20	001203-17-4	35
3			1,4,6,7-Tetramethyl1,2,3,4-tetra...	188	C14H20	1000113-61-3	27
4			1H-Inden-1-one, 2,3-dihydro-1,2,3...	188	C13H16O	089907-33-5	25
5			1,8-Naphthyridin-2-amine, 5,7-di...	173	C10H11N3	039565-07-6	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

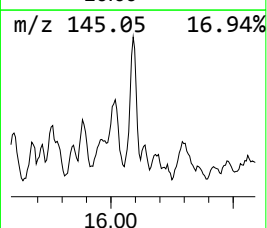
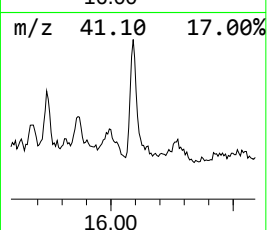
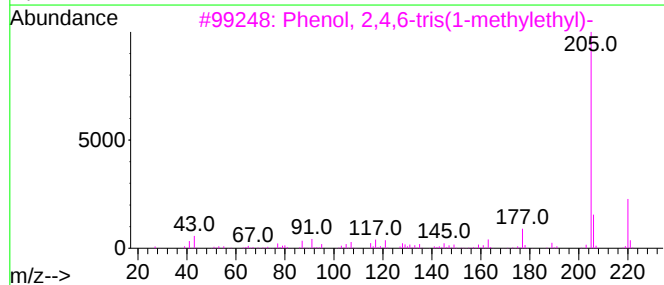
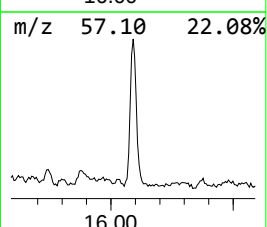
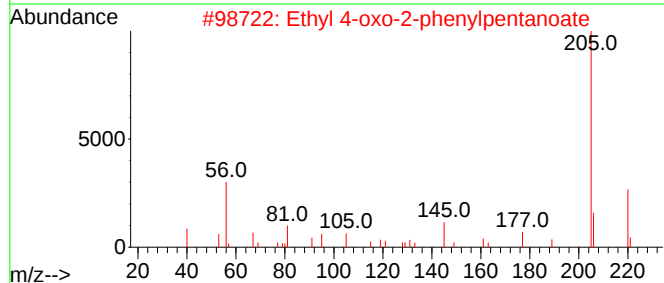
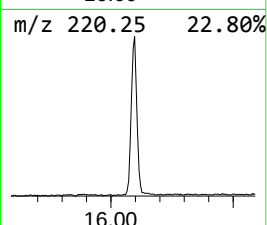
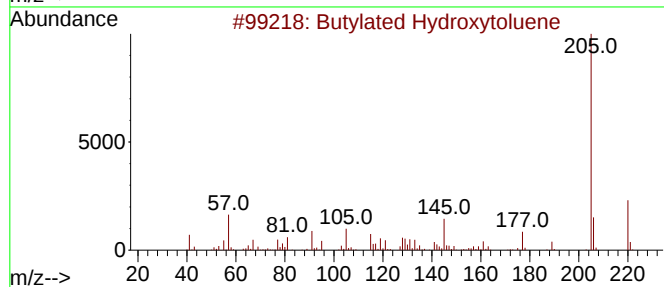
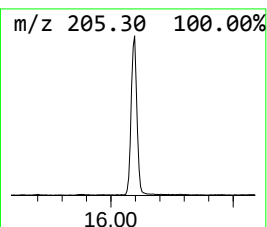
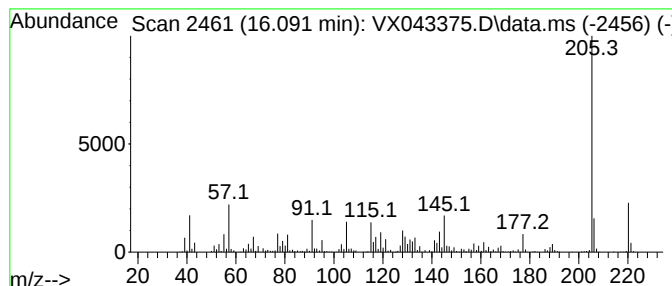
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Quant Title : SW846 8260

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

Peak Number 8 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.091	78.41 ug/l	563914	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	93
3			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	76
4			Phenol, 4,6-di(1,1-dimethylethyl)-	220	C15H24O	000616-55-7	70
5			2,4,6-Tris(1,1-dimethylethyl)-4-	276	C19H32O	019687-22-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

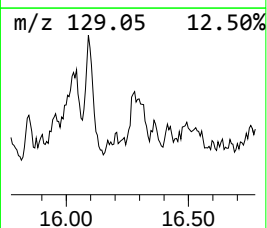
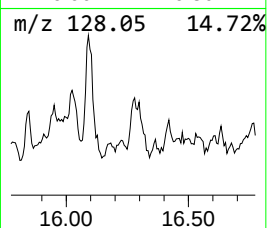
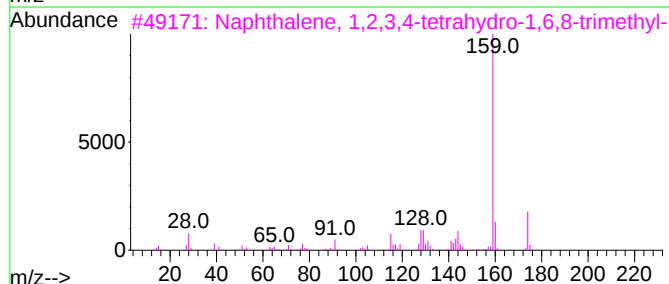
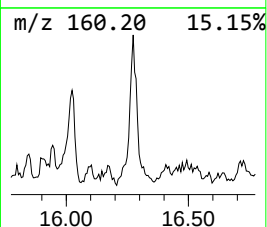
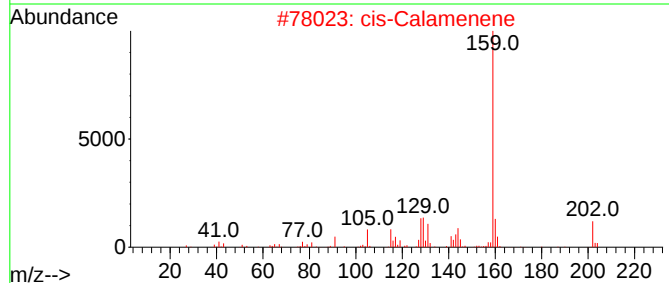
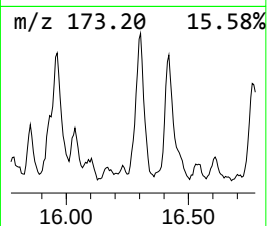
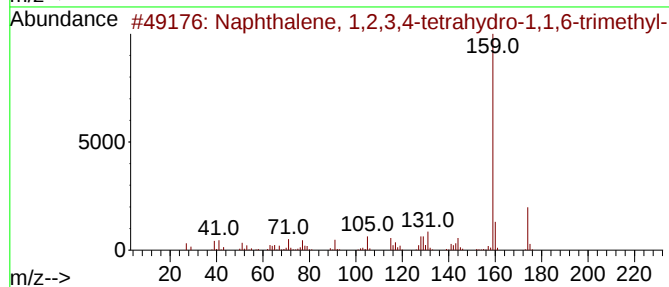
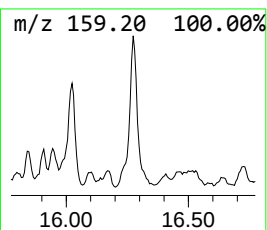
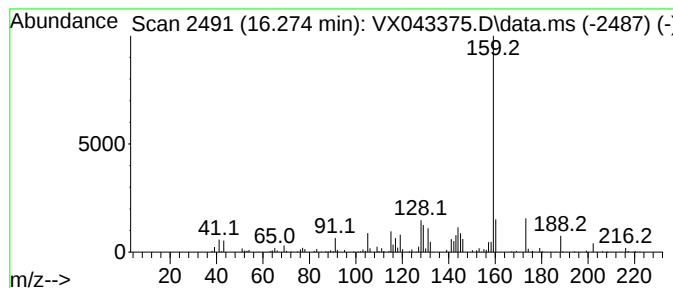
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Quant Title : SW846 8260

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

Peak Number 9 cis-Calamenene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.273	38.10 ug/l	274015	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	000475-03-6	87
2			cis-Calamenene	202	C15H22	072937-55-4	87
3			Naphthalene, 1,2,3,4-tetrahydro-...	174	C13H18	030316-36-0	87
4			Naphthalene, 1,2,3,4-tetrahydro-...	202	C15H22	000483-77-2	83
5			Benzene, 1-(1-formylethyl)-4-(1-...	188	C13H16O	1000161-46-6	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

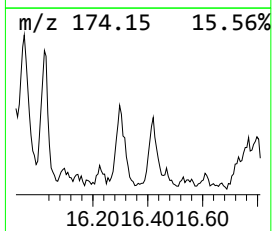
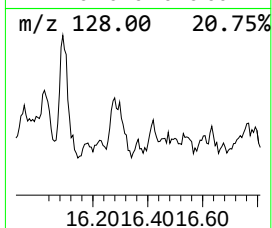
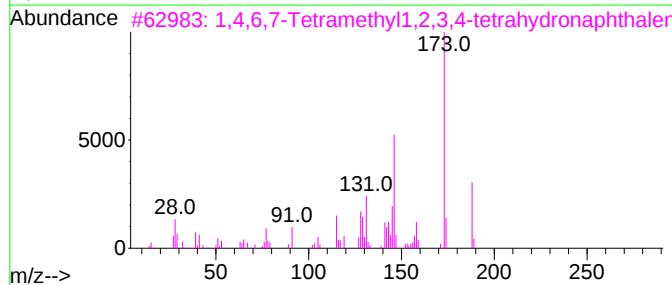
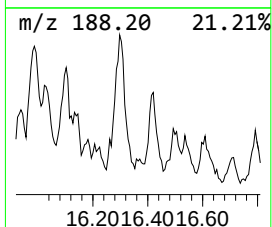
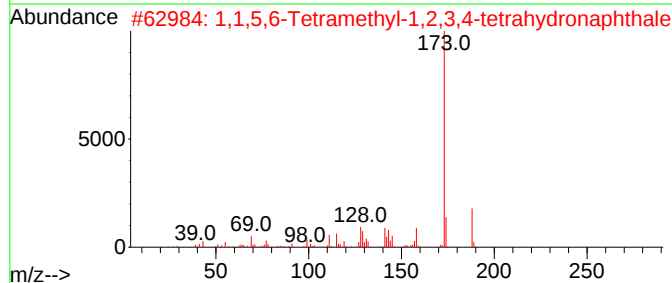
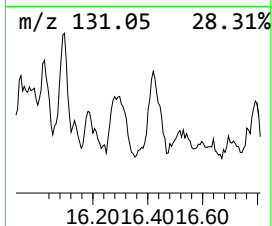
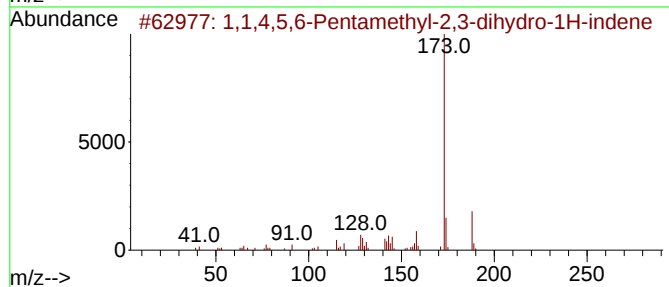
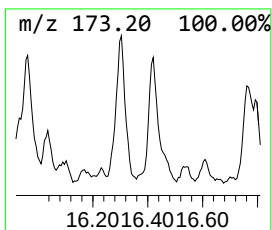
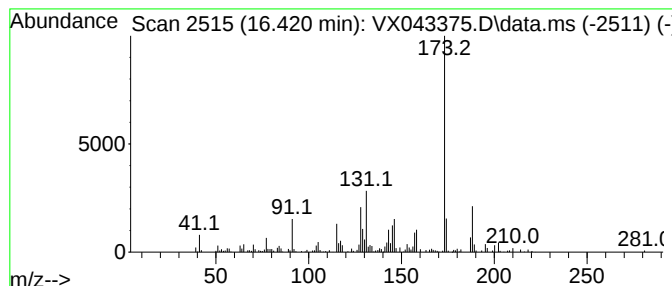
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

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

Peak Number 10 1,1,4,5,6-Pentamethyl-2,3-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.420	14.44 ug/l	103867	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4,5,6-Pentamethyl-2,3-dihydr...	188	C14H20	016204-67-4	76		
2	1,1,5,6-Tetramethyl-1,2,3,4-tetr...	188	C14H20	031197-54-3	68		
3	1,4,6,7-Tetramethyl-1,2,3,4-tetra...	188	C14H20	1000113-61-3	59		
4	Naphthalene, 6-(1,1-dimethylethy...	188	C14H20	042044-26-8	53		
5	5,8-Dimethyl-4-quinolinol	173	C11H11NO	203626-57-7	53		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101424\
Data File : VX043375.D
Acq On : 14 Oct 2024 12:12
Operator : JC/MD
Sample : P4394-01 20X
Misc : 1.50g/10mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WASH-DEBRIS

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100124W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, de...	13.414	12.9	ug/l	92385	4	12.024	359594	50.0
Naphthalene, 1,...	14.615	24.3	ug/l	174665	4	12.024	359594	50.0
Benzene, 1-(1-m...	14.670	11.8	ug/l	84997	4	12.024	359594	50.0
unknown14.847	14.847	13.1	ug/l	94352	4	12.024	359594	50.0
Ethanone, 1-[4-...	15.182	17.5	ug/l	125848	4	12.024	359594	50.0
Decahydro-1,1,4...	15.414	11.8	ug/l	84773	4	12.024	359594	50.0
unknown15.853	15.853	17.8	ug/l	128206	4	12.024	359594	50.0
Butylated Hydro...	16.091	78.4	ug/l	563914	4	12.024	359594	50.0
cis-Calamenene	16.273	38.1	ug/l	274015	4	12.024	359594	50.0
1,1,4,5,6-Penta...	16.420	14.4	ug/l	103867	4	12.024	359594	50.0