

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
 Data File : VX042914.D
 Acq On : 07 Aug 2024 14:38
 Operator : JC/MD
 Sample : P3462-01
 Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 JC-1

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\82X080724W.M
 Title : SW846 8260

Signal : TIC: VX042914.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	694	706	721	rBV2	79460	281428	5.98%	1.842%
2	5.544	721	731	751	rVB2	160819	474518	10.08%	3.106%
3	5.952	790	798	807	rBV	103952	282208	5.99%	1.847%
4	6.757	921	930	947	rBV	260320	650262	13.81%	4.256%
5	8.647	1234	1240	1247	rBV	523870	807782	17.16%	5.287%
6	8.720	1247	1252	1258	rVB	97896	157399	3.34%	1.030%
7	8.909	1278	1283	1290	rBV	41943	61301	1.30%	0.401%
8	9.903	1442	1446	1458	rVB3	32292	51216	1.09%	0.335%
9	10.055	1466	1471	1487	rVB	568144	812562	17.26%	5.319%
10	10.195	1487	1494	1502	rVV	75833	112710	2.39%	0.738%
11	10.299	1503	1511	1517	rVV	365300	529739	11.25%	3.467%
12	10.360	1517	1521	1531	rVB	121200	159755	3.39%	1.046%
13	10.640	1562	1567	1576	rBV	174365	257976	5.48%	1.689%
14	11.086	1634	1640	1649	rBV	444637	653919	13.89%	4.280%
15	11.378	1684	1688	1695	rVV	94382	173947	3.69%	1.139%
16	11.451	1695	1700	1702	rVV	122512	173443	3.68%	1.135%
17	11.476	1702	1704	1709	rVB	166278	178787	3.80%	1.170%
18	11.616	1718	1727	1733	rBV	38502	73166	1.55%	0.479%
19	11.750	1745	1749	1757	rVB	215936	278386	5.91%	1.822%
20	12.024	1788	1794	1800	rBV	586815	795321	16.89%	5.206%
21	12.085	1800	1804	1810	rVB	113374	171349	3.64%	1.122%
22	12.244	1823	1830	1832	rBV3	28872	50274	1.07%	0.329%
23	12.317	1838	1842	1849	rVB3	59208	95624	2.03%	0.626%
24	12.421	1852	1859	1863	rBV2	184956	253336	5.38%	1.658%
25	12.963	1944	1948	1956	rVB	66547	108100	2.30%	0.708%
26	13.268	1993	1998	1999	rBV	67174	81221	1.73%	0.532%
27	13.286	1999	2001	2007	rVB2	62465	98865	2.10%	0.647%
28	13.427	2019	2024	2033	rVB8	44072	95691	2.03%	0.626%
29	13.774	2072	2081	2088	rBV	3900990	4707713	100.00%	30.814%
30	13.872	2093	2097	2100	rVB	49440	69128	1.47%	0.452%
31	14.219	2148	2154	2159	rVB6	36784	56126	1.19%	0.367%
32	14.634	2215	2222	2227	rBV	665853	830298	17.64%	5.435%
33	14.780	2239	2246	2254	rVB	471770	647605	13.76%	4.239%
34	15.207	2308	2316	2320	rBV	91755	147775	3.14%	0.967%
35	15.377	2339	2344	2347	rBV2	40842	61514	1.31%	0.403%
36	15.475	2355	2360	2368	rBV2	139747	250837	5.33%	1.642%

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Integrator: RTE

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37	15.609	2377	2382	2386	rBV	157063	254160	5.40%	1.664%
38	15.646	2386	2388	2397	rVB	97846	142372	3.02%	0.932%
39	15.835	2411	2419	2423	rBV3	39033	96123	2.04%	0.629%
40	16.085	2455	2460	2468	rBV4	46236	93753	1.99%	0.614%

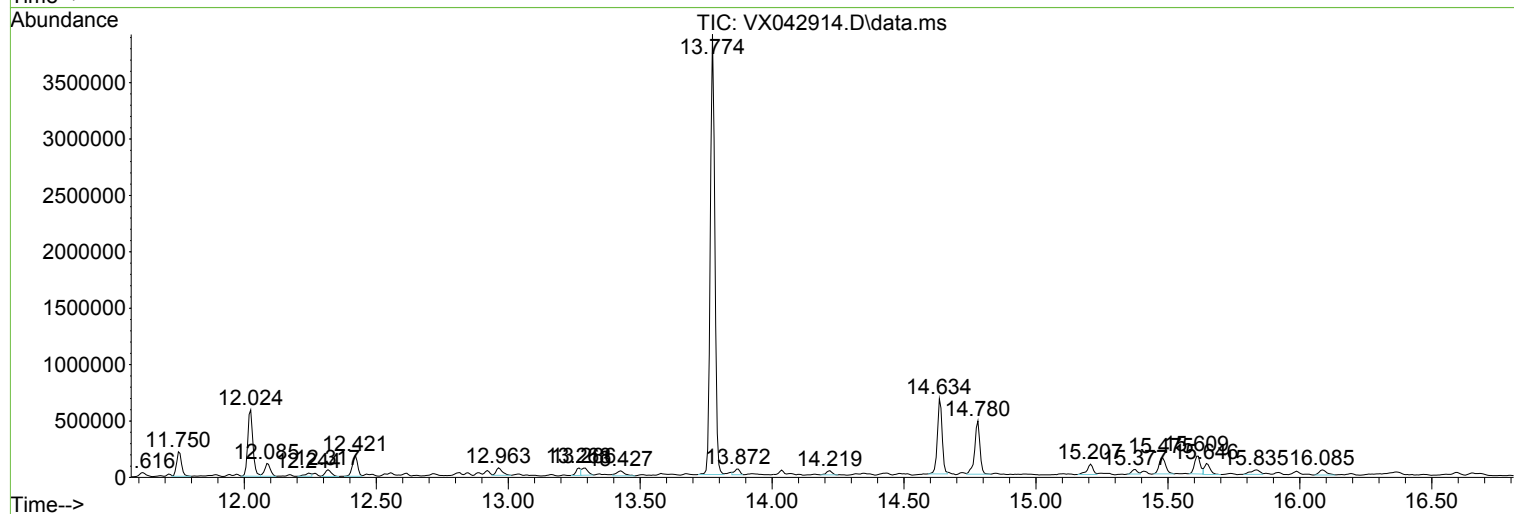
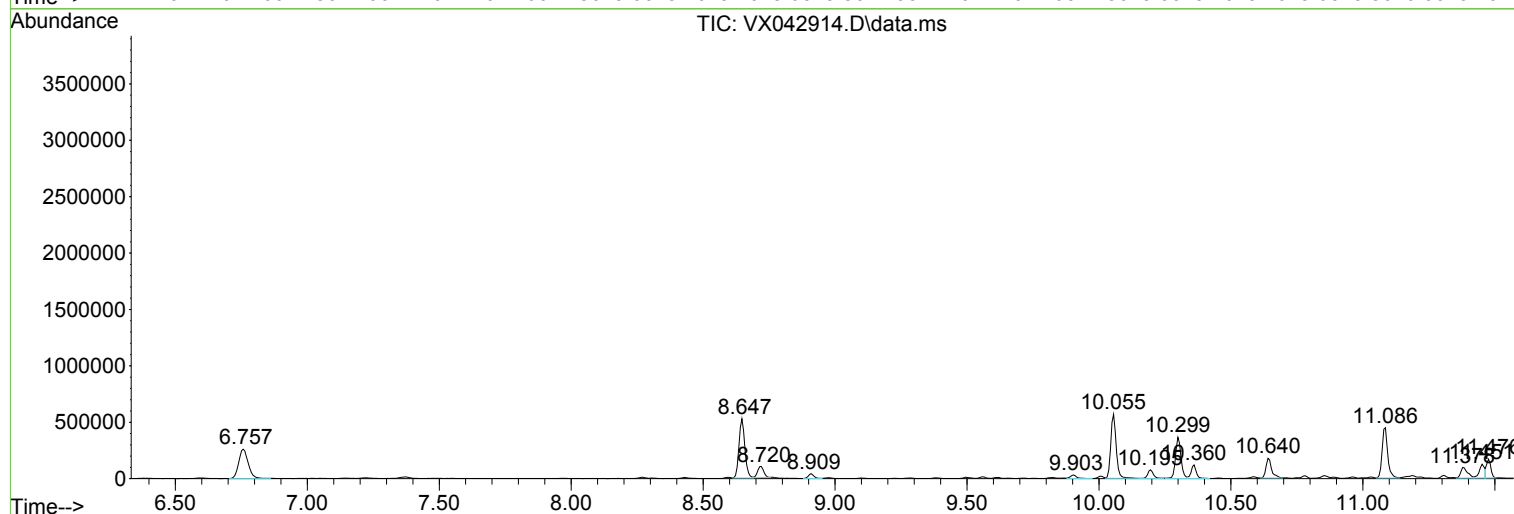
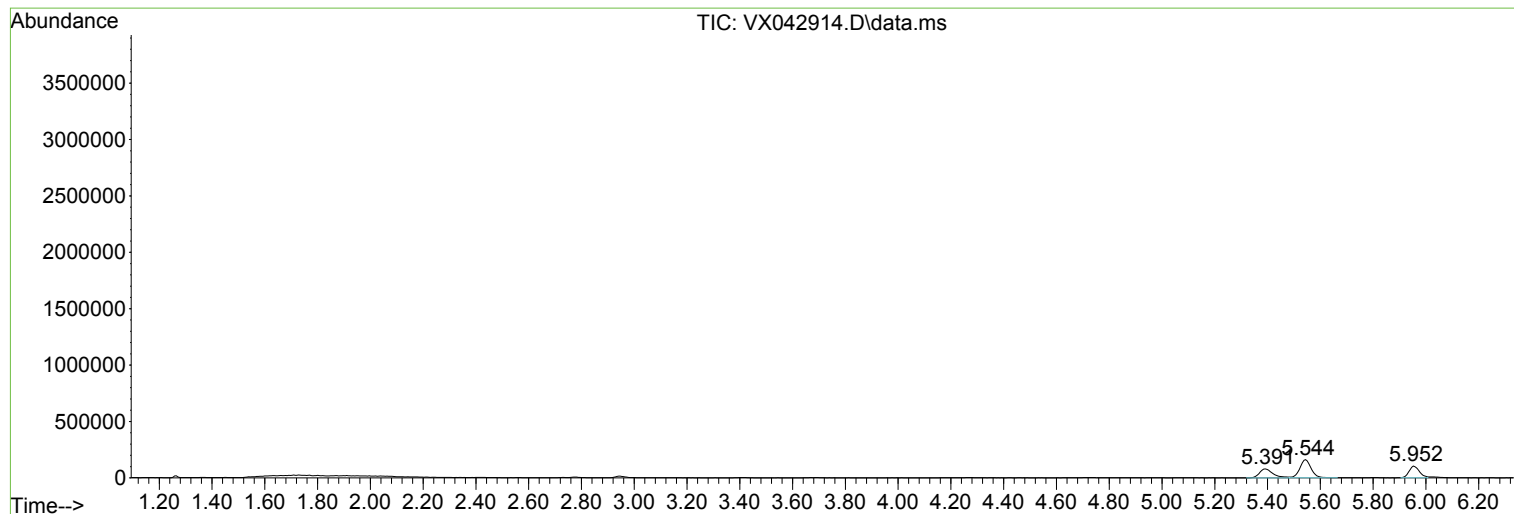
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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



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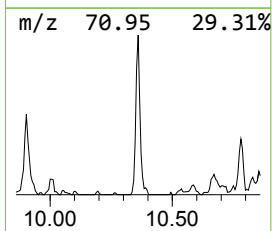
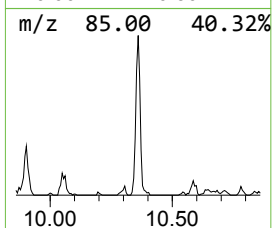
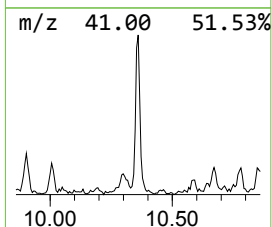
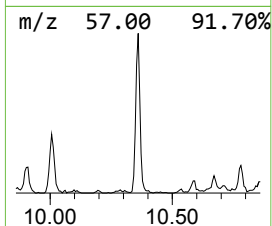
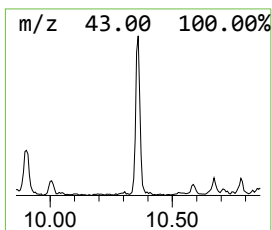
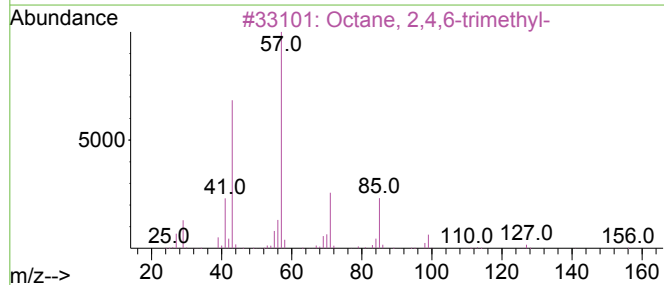
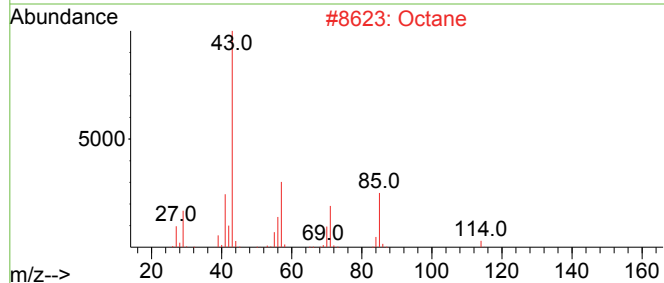
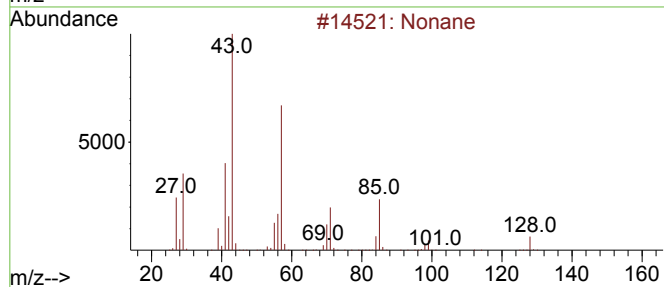
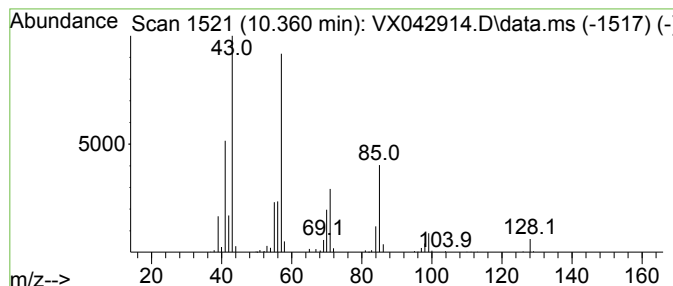
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 1 Nonane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.360	9.83 ug/l	159755	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonane	128	C9H20	000111-84-2	95
2			Octane	114	C8H18	000111-65-9	64
3			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64
4			Sulfurous acid, hexyl pentadecyl...	376	C21H44O3S	1000309-13-7	59
5			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

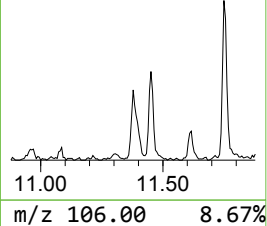
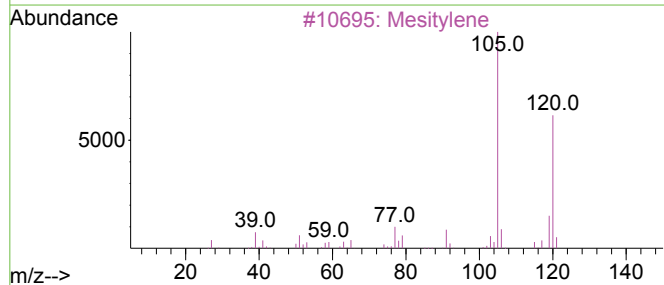
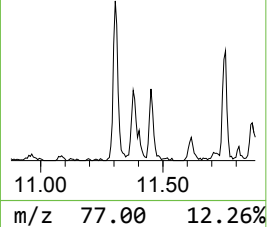
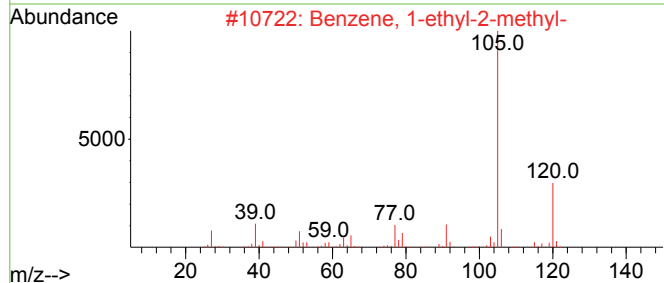
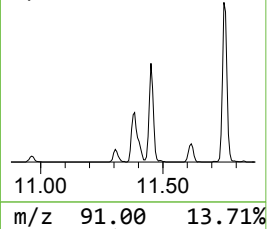
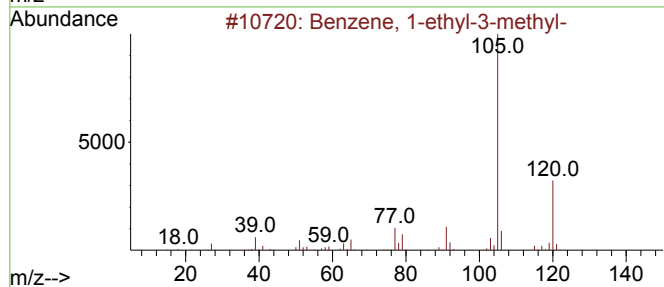
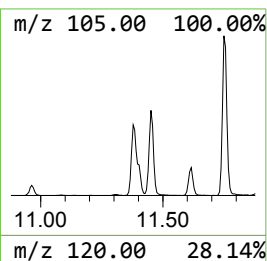
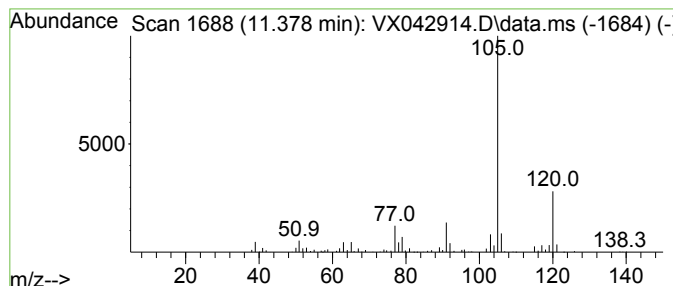
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	10.94 ug/l	173947	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

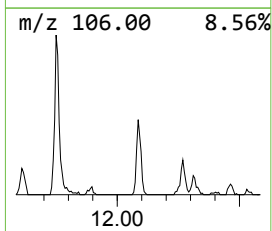
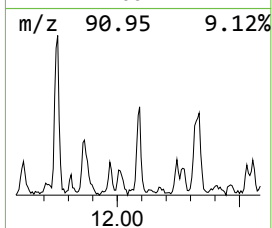
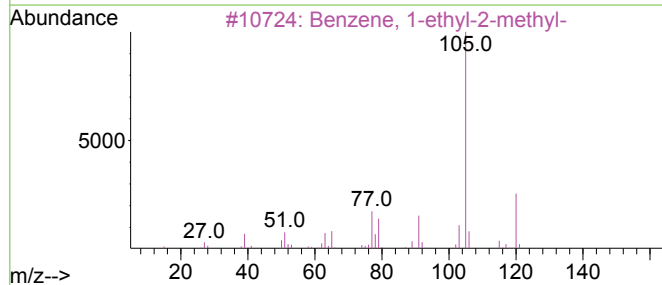
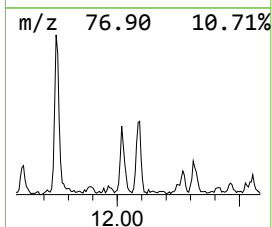
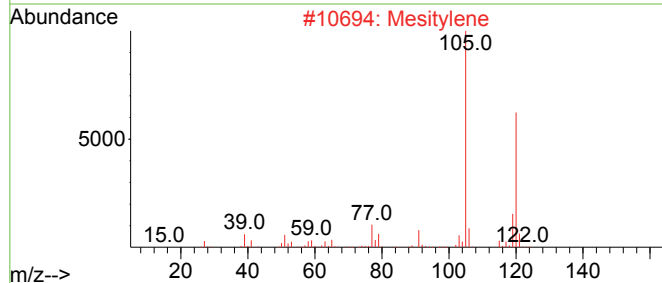
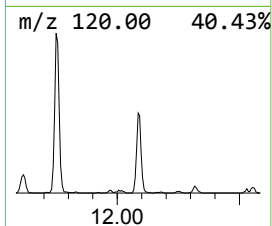
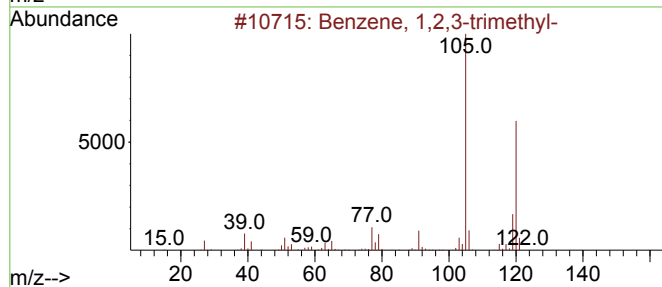
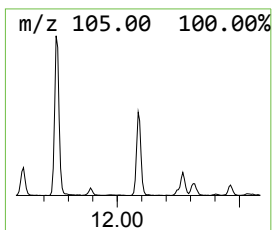
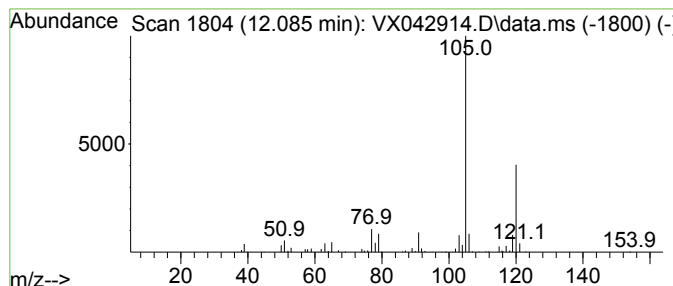
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.085	10.77 ug/l	171349	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2			Mesitylene	120	C9H12	000108-67-8	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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ALS Vial : 13 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
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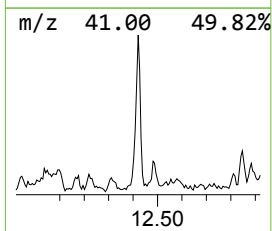
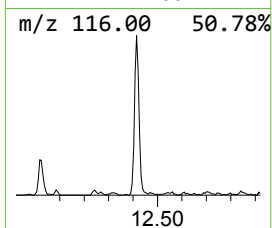
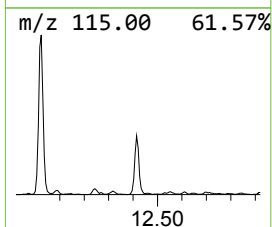
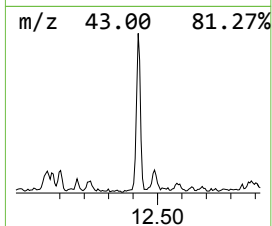
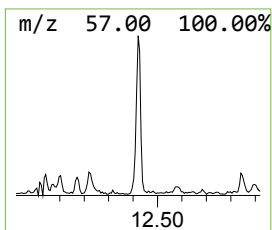
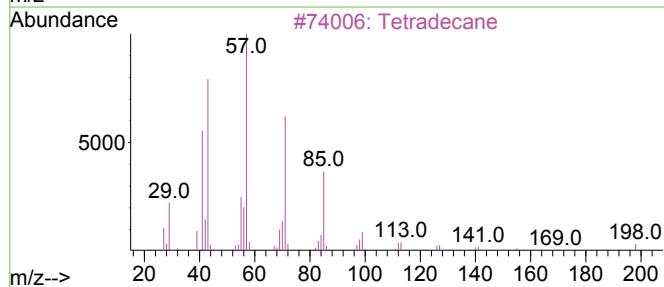
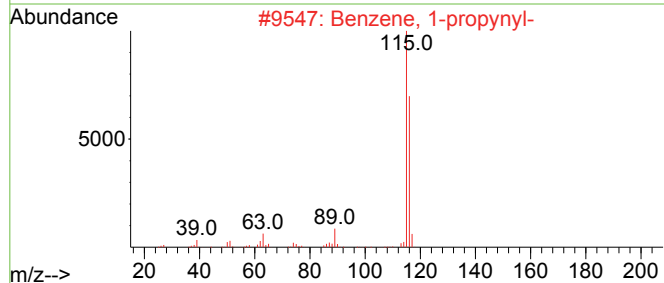
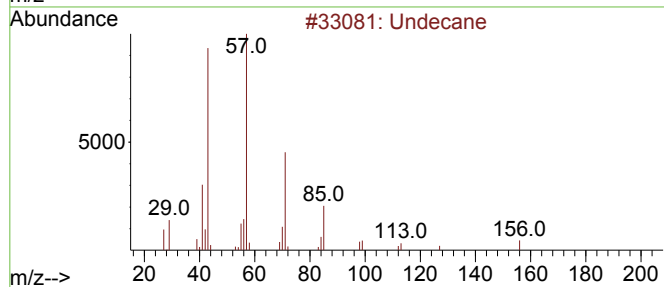
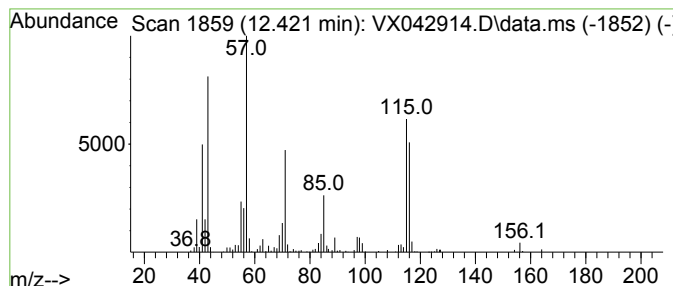
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Peak Number 4 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	15.93 ug/l	253336	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	89
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	46
3			Tetradecane	198	C14H30	000629-59-4	43
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	41
5			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	41



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MSVOA_X
ClientSampleId :
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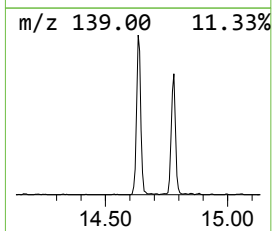
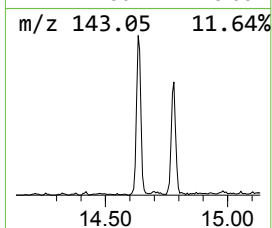
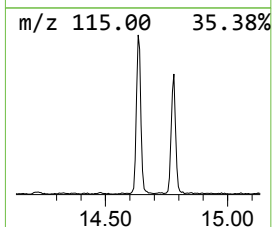
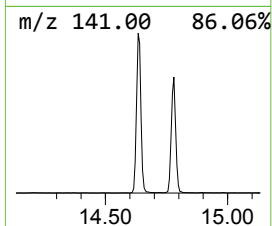
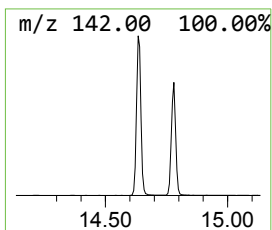
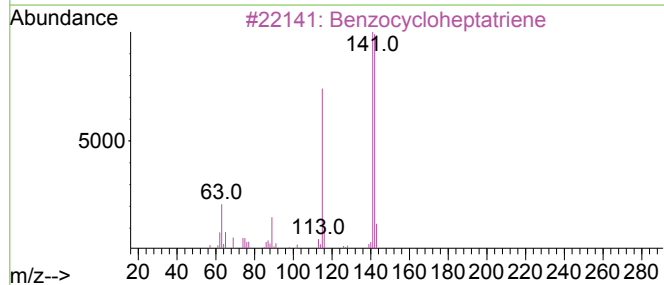
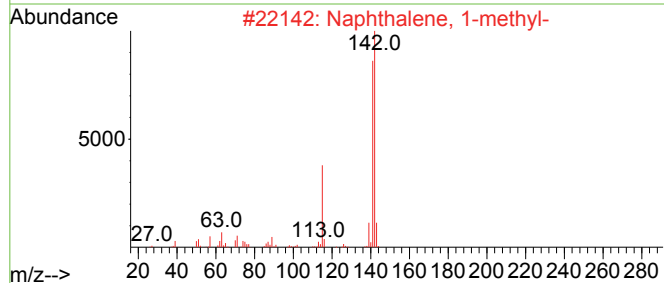
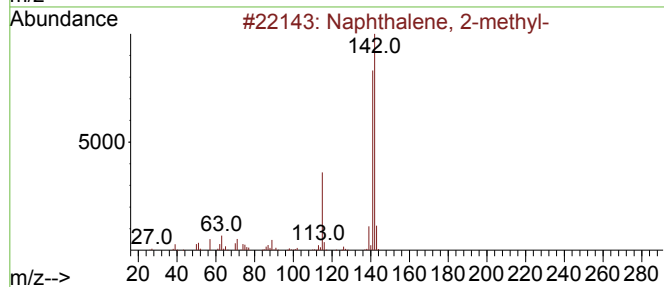
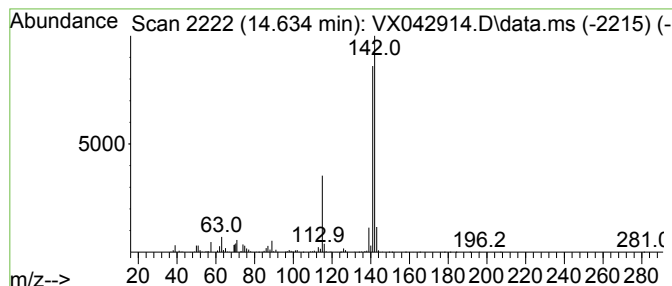
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	52.20 ug/l	830298	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

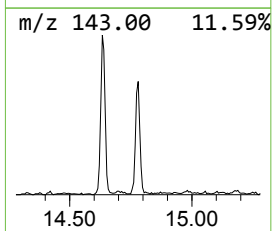
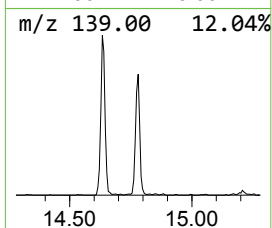
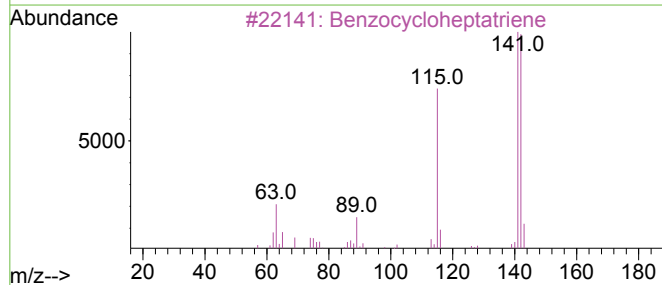
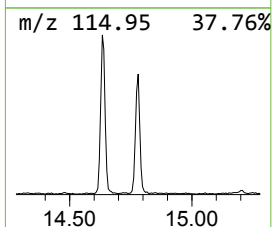
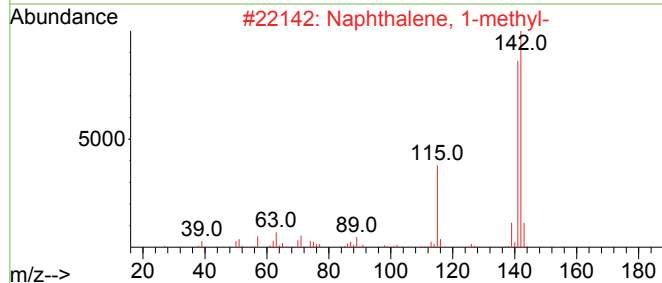
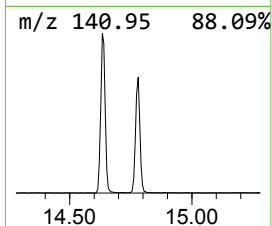
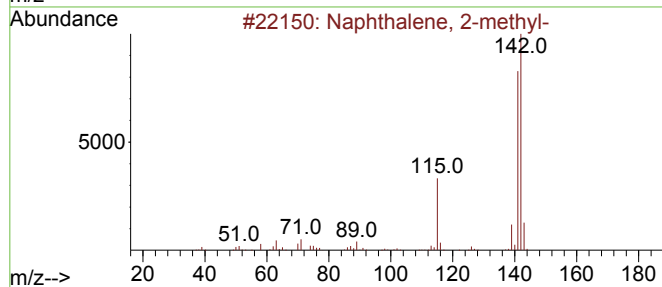
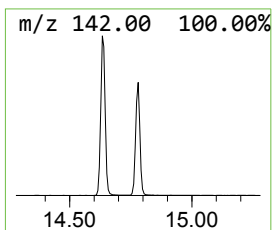
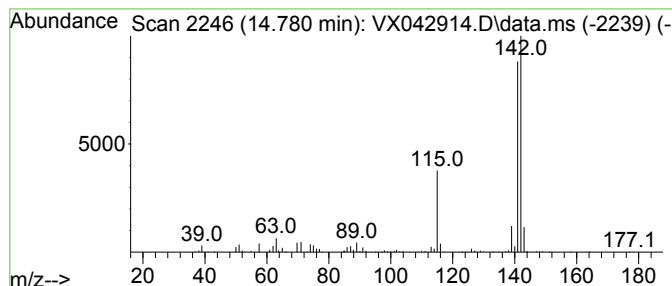
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	40.71 ug/l	647605	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

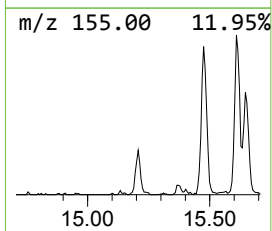
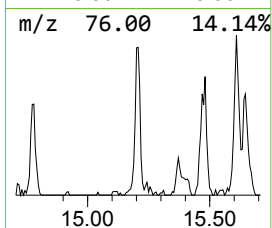
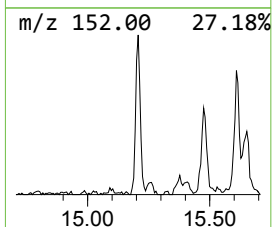
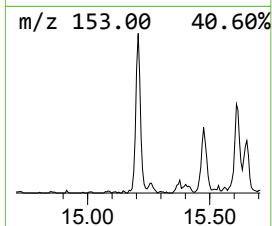
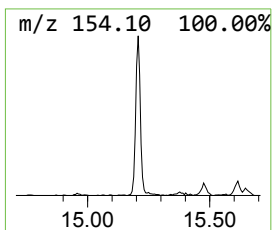
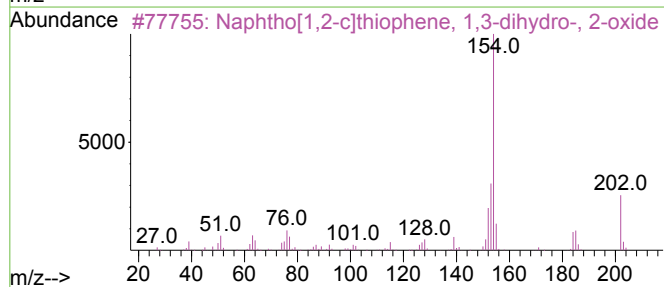
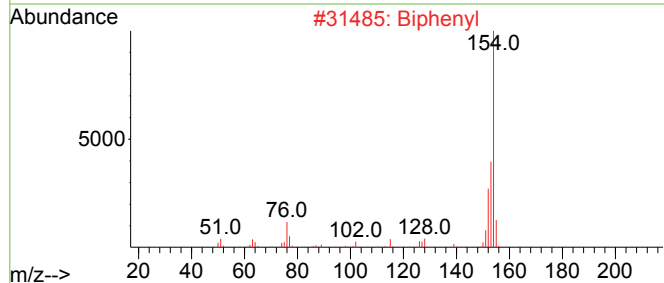
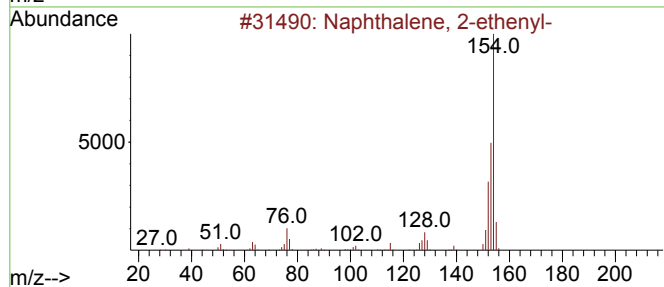
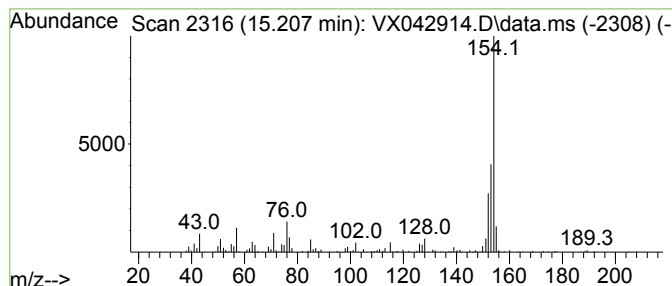
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2-ethenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.207	9.29 ug/l	147775	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	94
2			Biphenyl	154	C12H10	000092-52-4	94
3			Naphtho[1,2-c]thiophene, 1,3-dih...	202	C12H10S	031739-49-8	83
4			1-(2,2-Difluoroethenyl)-4-methyl...	154	C9H8F2	1000305-64-2	59
5			1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

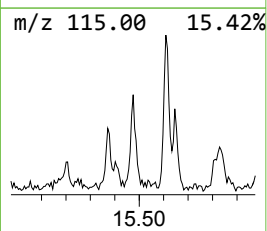
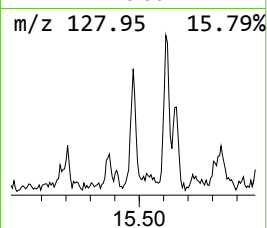
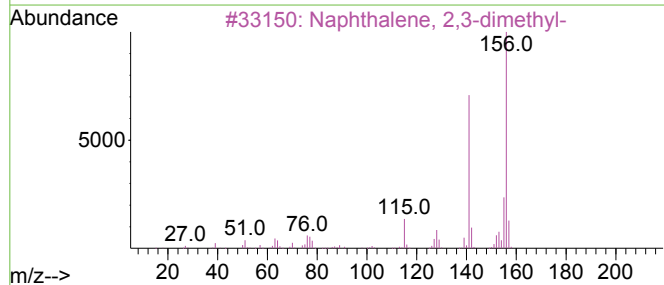
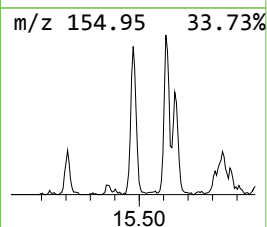
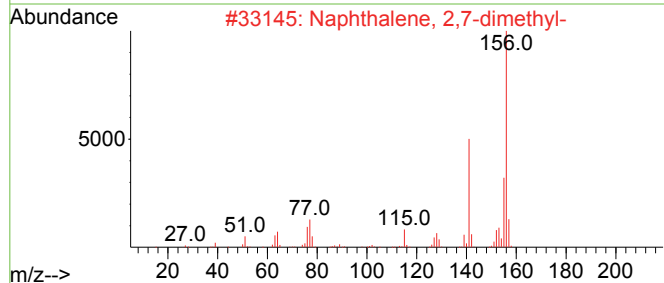
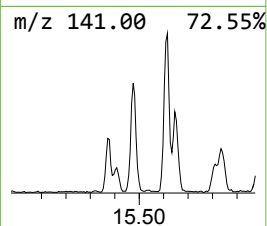
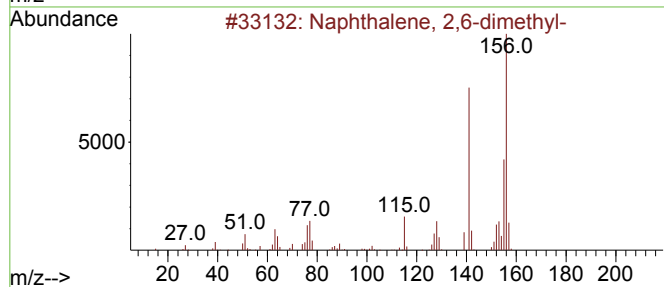
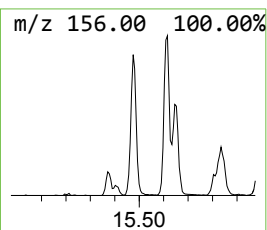
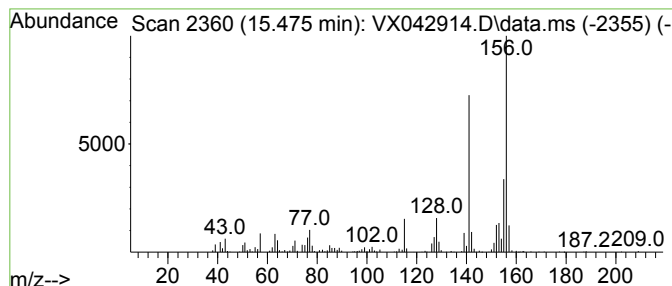
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Quant Title : SW846 8260

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

Peak Number 8 Naphthalene, 2,6-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.475	15.77 ug/l	250837	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
2			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

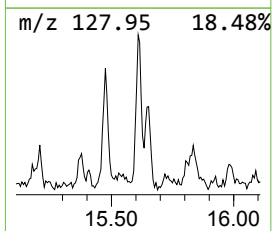
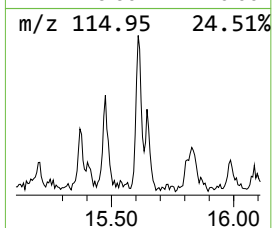
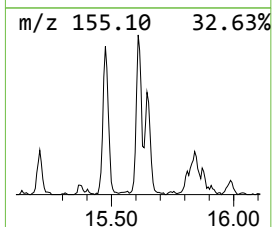
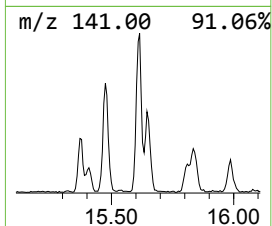
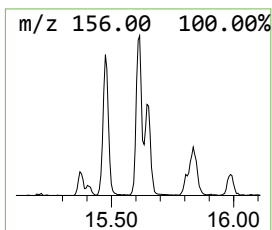
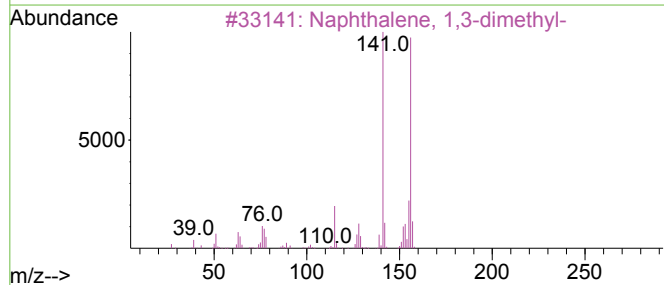
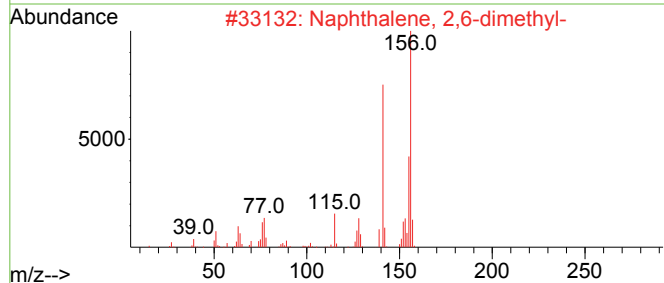
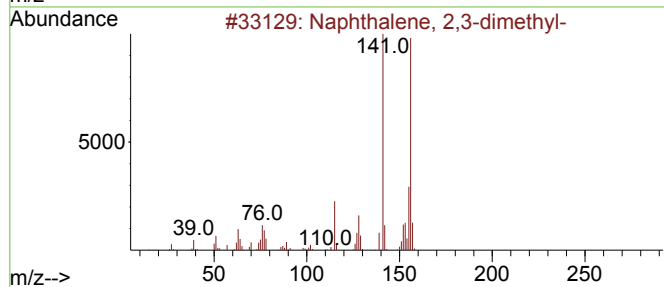
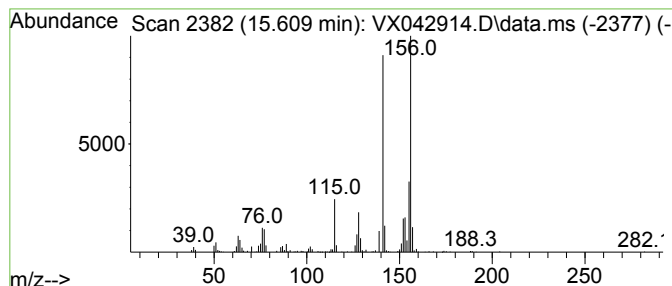
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.609	15.98 ug/l	254160	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

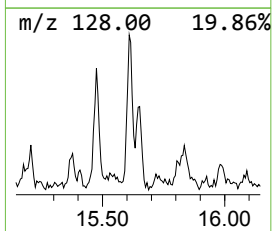
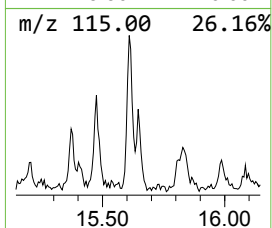
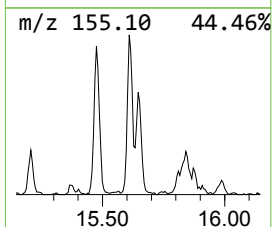
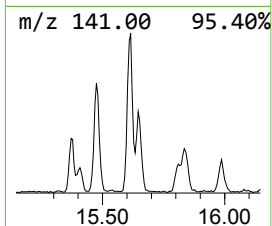
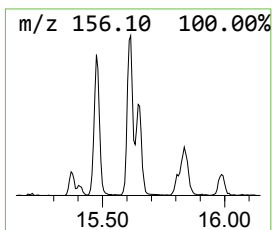
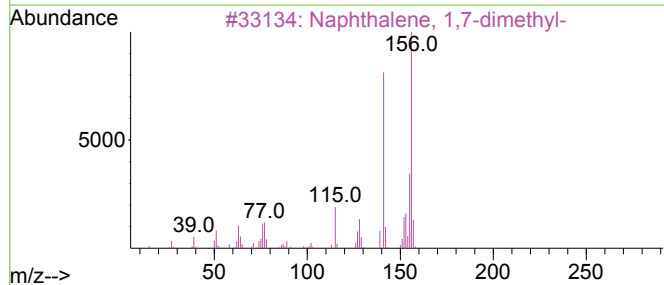
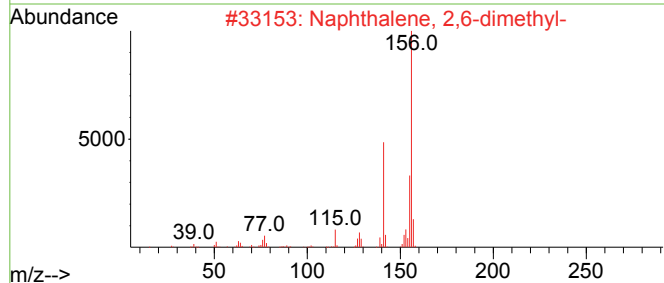
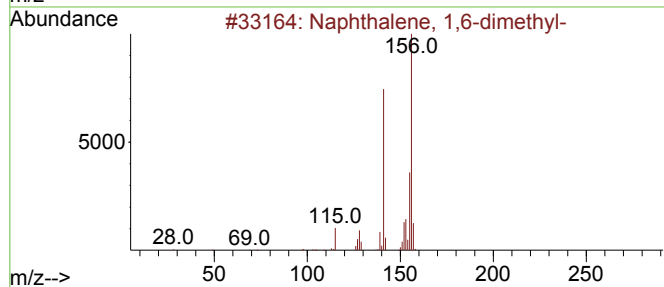
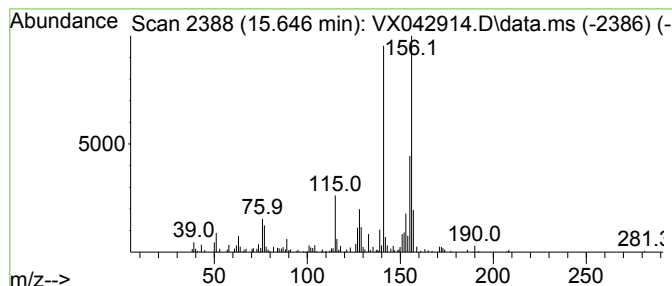
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Quant Title : SW846 8260

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

Peak Number 10 Naphthalene, 1,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.646	8.95 ug/l	142372	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	94
3			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042914.D
Acq On : 07 Aug 2024 14:38
Operator : JC/MD
Sample : P3462-01
Misc : 5.00g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.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
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Benzene, 1-ethy...	11.378	10.9	ug/l	173947	4	12.024	795321	50.0
Benzene, 1,2,3-...	12.085	10.8	ug/l	171349	4	12.024	795321	50.0
Undecane	12.421	15.9	ug/l	253336	4	12.024	795321	50.0
Naphthalene, 2-...	14.634	52.2	ug/l	830298	4	12.024	795321	50.0
Naphthalene, 1-...	14.780	40.7	ug/l	647605	4	12.024	795321	50.0
Naphthalene, 2-...	15.207	9.3	ug/l	147775	4	12.024	795321	50.0
Naphthalene, 2,...	15.475	15.8	ug/l	250837	4	12.024	795321	50.0
Naphthalene, 2,...	15.609	16.0	ug/l	254160	4	12.024	795321	50.0
Naphthalene, 1,...	15.646	8.9	ug/l	142372	4	12.024	795321	50.0