

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
 Data File : VX042909.D
 Acq On : 07 Aug 2024 12:41
 Operator : JC/MD
 Sample : P3462-05
 Misc : 5.04g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 JC-2

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: VX042909.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	37	rBV	15069	17704	1.81%	0.201%
2	1.624	69	88	89	rBV6	16104	68604	7.00%	0.778%
3	2.947	296	305	314	rBV2	9694	25124	2.56%	0.285%
4	5.385	693	705	718	rBV2	102858	309094	31.52%	3.505%
5	5.544	721	731	744	rVV2	161836	463365	47.26%	5.254%
6	5.952	788	798	807	rBV	110853	297060	30.30%	3.369%
7	6.025	808	810	828	rVB4	12387	29165	2.97%	0.331%
8	6.757	919	930	954	rBV	276708	674210	68.76%	7.645%
9	7.220	1000	1006	1016	rVB4	4513	12021	1.23%	0.136%
10	8.647	1234	1240	1248	rBV	583841	922535	94.09%	10.461%
11	8.720	1248	1252	1270	rVB	41295	85499	8.72%	0.970%
12	10.055	1465	1471	1488	rVB	607819	846779	86.36%	9.602%
13	10.195	1488	1494	1502	rVB	10858	16279	1.66%	0.185%
14	10.299	1504	1511	1517	rBV	68245	103726	10.58%	1.176%
15	10.360	1517	1521	1526	rVB4	9593	14697	1.50%	0.167%
16	10.640	1563	1567	1577	rBV	48056	75890	7.74%	0.861%
17	11.085	1633	1640	1651	rBV	488098	676775	69.03%	7.674%
18	11.378	1683	1688	1696	rVV	19743	42024	4.29%	0.477%
19	11.451	1696	1700	1703	rVV	37537	56711	5.78%	0.643%
20	11.475	1703	1704	1710	rVB	22646	21102	2.15%	0.239%
21	11.616	1721	1727	1733	rBV	11316	19146	1.95%	0.217%
22	11.750	1745	1749	1757	rVB	72569	93455	9.53%	1.060%
23	12.024	1788	1794	1800	rBV	617348	808998	82.51%	9.174%
24	12.091	1800	1805	1809	rVB	33855	51729	5.28%	0.587%
25	12.244	1823	1830	1833	rBV5	10310	18442	1.88%	0.209%
26	12.317	1838	1842	1849	rBV2	15229	24780	2.53%	0.281%
27	12.420	1852	1859	1864	rVV2	48048	72515	7.40%	0.822%
28	12.469	1864	1867	1873	rVB7	5453	10414	1.06%	0.118%
29	12.555	1874	1881	1885	rBV6	8042	19989	2.04%	0.227%
30	12.817	1917	1924	1926	rBV6	7382	12254	1.25%	0.139%
31	12.920	1938	1941	1944	rVB3	8630	10018	1.02%	0.114%
32	12.963	1944	1948	1956	rVB4	15563	26069	2.66%	0.296%
33	13.268	1993	1998	2000	rBV	23824	31856	3.25%	0.361%
34	13.292	2000	2002	2008	rVB4	19523	23885	2.44%	0.271%
35	13.426	2014	2024	2033	rVB4	12679	35002	3.57%	0.397%
36	13.774	2076	2081	2088	rVB	814810	980477	100.00%	11.118%

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ClientSampleId :
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Integration Parameters: RTEINT.P

Integrator: RTE

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Filtering: 5

Sampling : 1

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Stop Thrs : 0

Peak Location: TOP

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

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37	13.871	2094	2097	2101	rVB	14359	16364	1.67%	0.186%
38	14.036	2118	2124	2128	rBV	18921	25852	2.64%	0.293%
39	14.219	2149	2154	2158	rBV5	9914	13527	1.38%	0.153%
40	14.414	2183	2186	2193	rBV6	6630	11808	1.20%	0.134%
41	14.633	2214	2222	2232	rVB	314340	421306	42.97%	4.777%
42	14.780	2239	2246	2253	rVB	246725	343701	35.05%	3.897%
43	15.207	2312	2316	2321	rVV2	42306	56063	5.72%	0.636%
44	15.274	2325	2327	2331	rVB5	10334	11859	1.21%	0.134%
45	15.371	2339	2343	2347	rBV	31253	44683	4.56%	0.507%
46	15.408	2347	2349	2355	rVB6	18763	26764	2.73%	0.303%
47	15.481	2355	2361	2369	rBV2	108802	205987	21.01%	2.336%
48	15.615	2377	2383	2386	rBV	120594	195201	19.91%	2.214%
49	15.652	2386	2389	2398	rVB	69617	105764	10.79%	1.199%
50	15.743	2400	2404	2410	rVB7	8175	13986	1.43%	0.159%
51	15.834	2410	2419	2429	rBV2	32463	93905	9.58%	1.065%
52	15.908	2429	2431	2437	rVB7	6978	11695	1.19%	0.133%
53	15.981	2439	2443	2449	rBV3	21872	35877	3.66%	0.407%
54	16.084	2455	2460	2468	rBV6	25694	59043	6.02%	0.670%
55	16.194	2474	2478	2484	rVB5	11047	20316	2.07%	0.230%
56	16.267	2484	2490	2491	rBV6	6677	11044	1.13%	0.125%
57	16.353	2497	2504	2505	rBV5	10597	20574	2.10%	0.233%
58	16.371	2505	2507	2512	rVB5	16263	20522	2.09%	0.233%
59	16.590	2540	2543	2549	rVB4	18505	30493	3.11%	0.346%
60	16.657	2549	2554	2556	rBV3	14390	24928	2.54%	0.283%

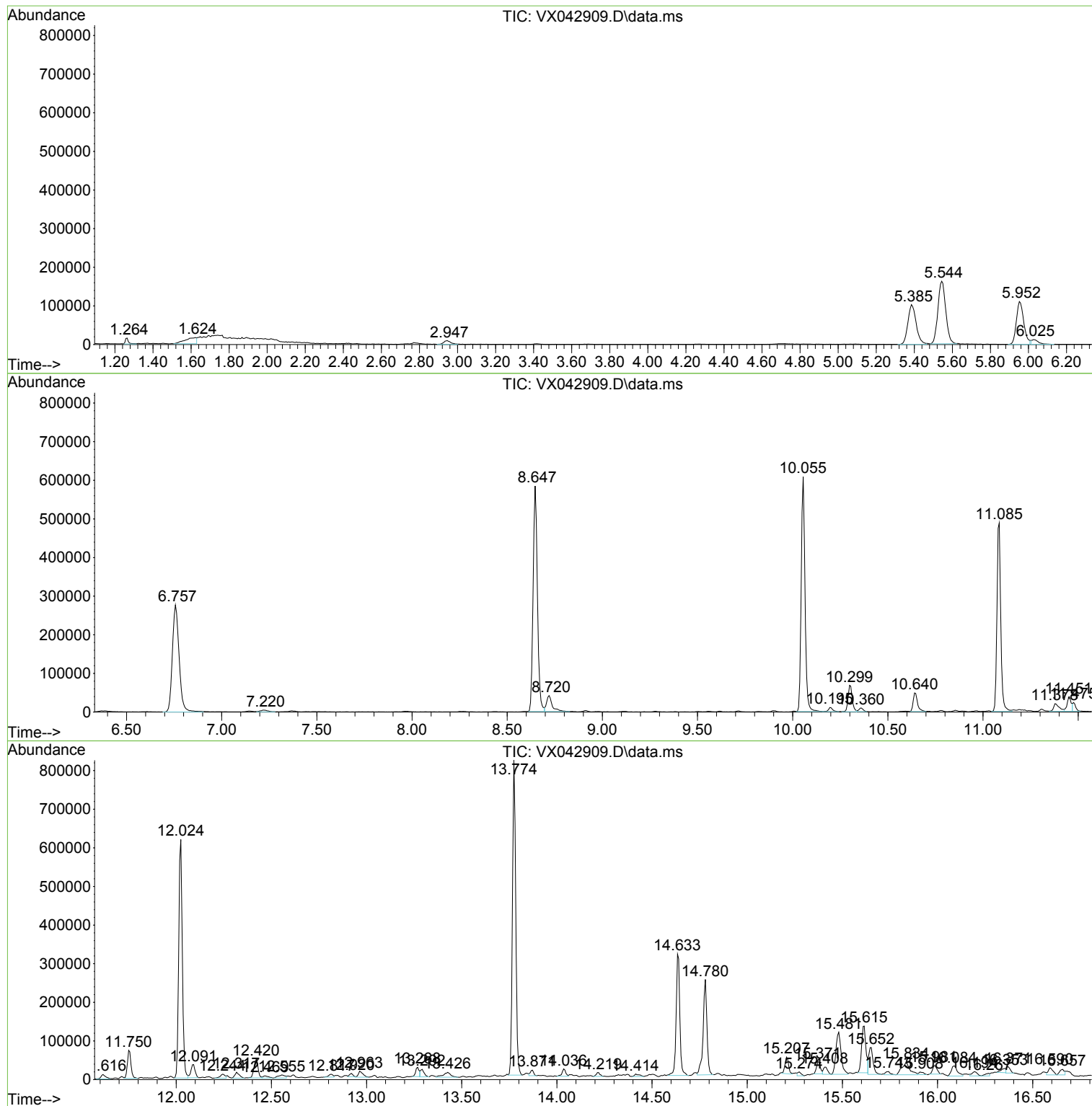
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Quant Title : SW846 8260

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



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ALS Vial : 8 Sample Multiplier: 1

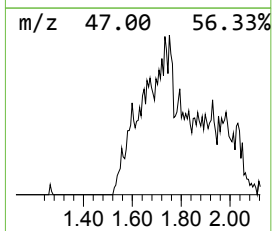
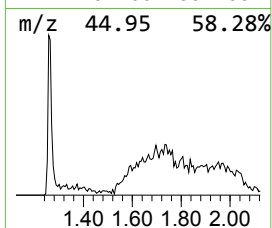
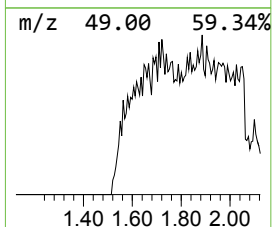
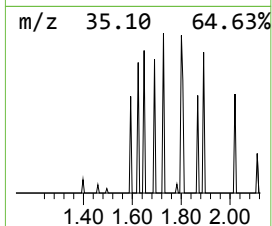
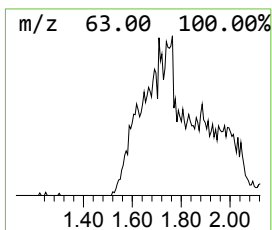
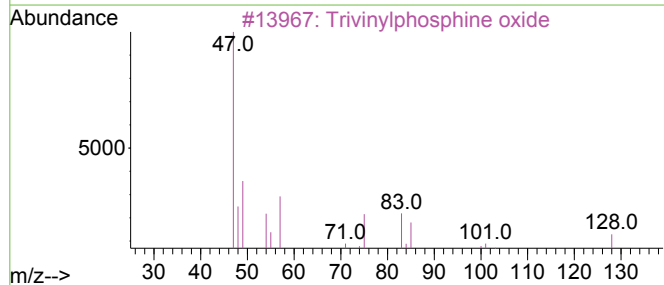
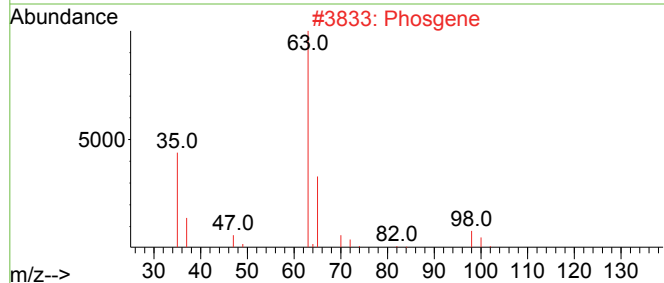
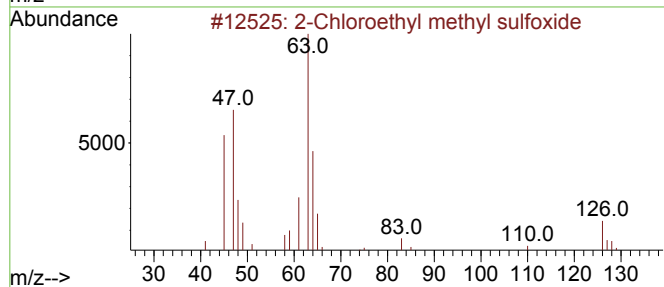
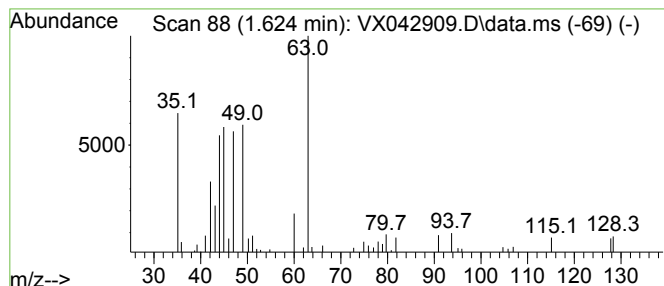
Instrument :
MSVOA_X
ClientSampleId :
JC-2

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 unknown1.624 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.624	7.40 ug/l	68604	Pentafluorobenzene	5.550	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	33
2	Phosgene	98	CCl2O	000075-44-5	9
3	Trivinylphosphine oxide	128	C6H9OP	013699-67-7	5
4	Methan-d3-ol	35	CHD3O	001849-29-2	4
5	Ethene, trifluoro-	82	C2HF3	000359-11-5	4



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-2

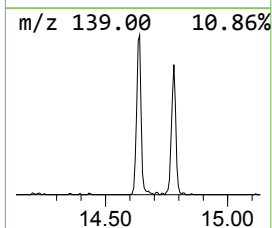
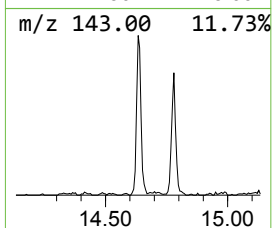
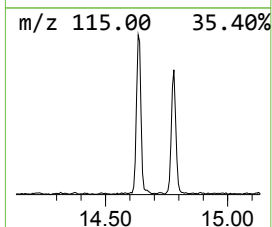
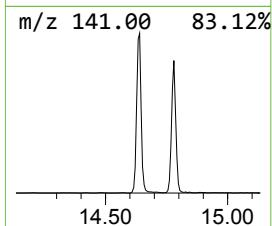
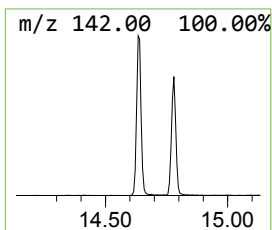
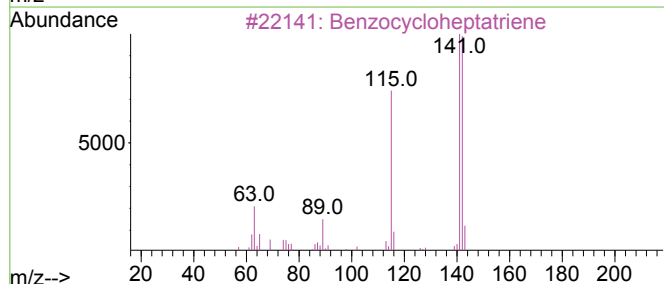
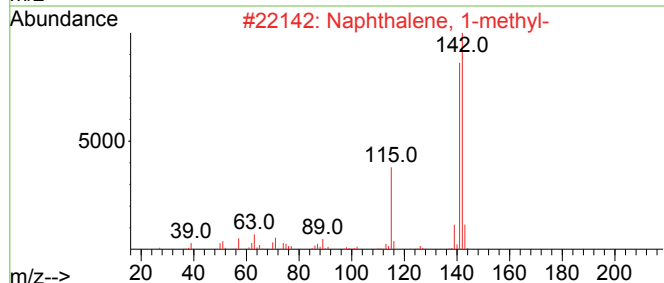
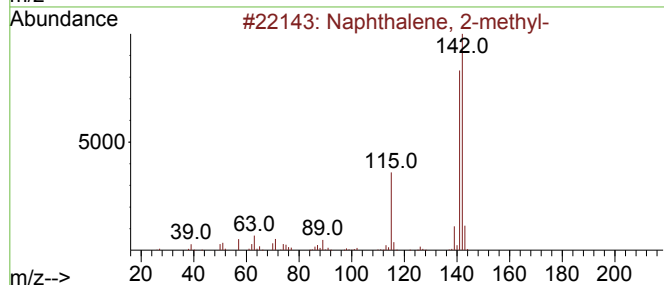
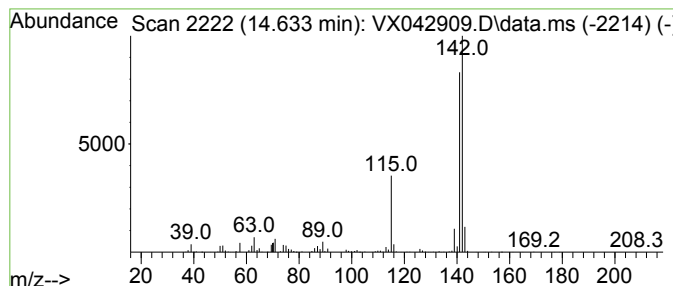
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.634	26.04 ug/l	421306	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	78
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
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Sample : P3462-05
Misc : 5.04g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

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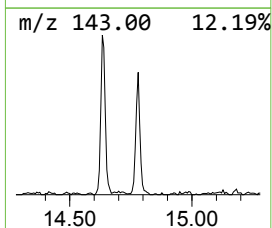
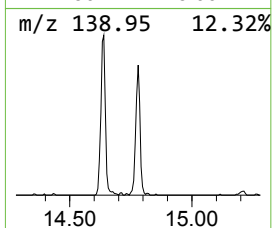
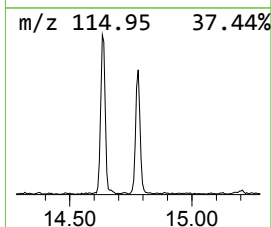
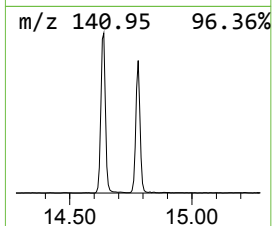
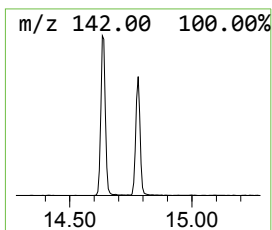
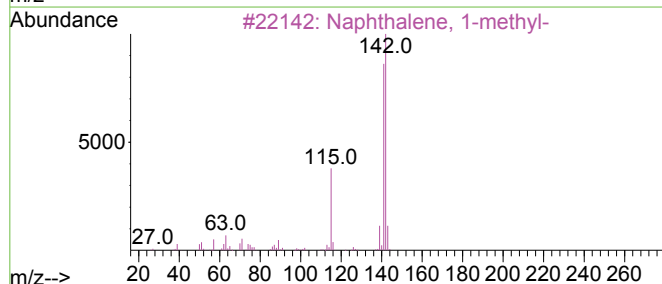
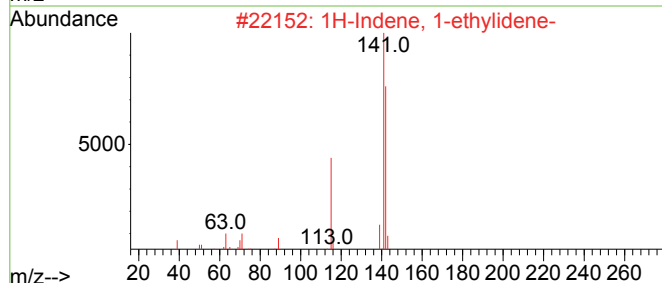
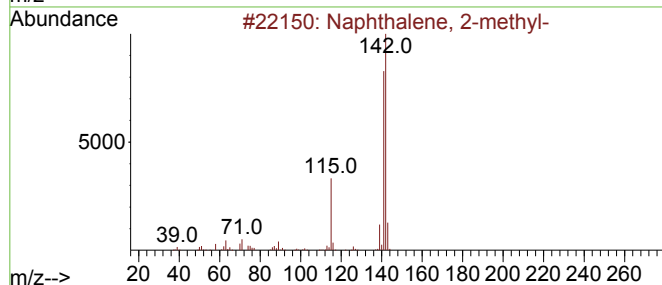
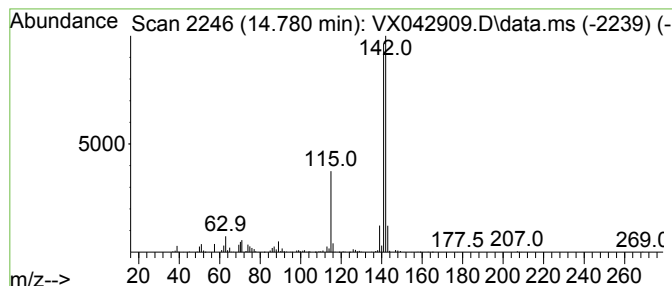
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 3 1H-Indene, 1-ethylidene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	21.24 ug/l	343701	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	95
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5			Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91



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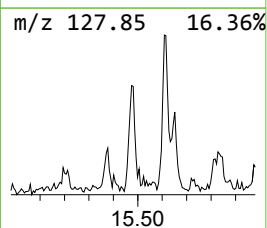
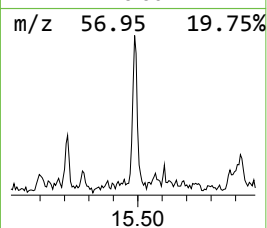
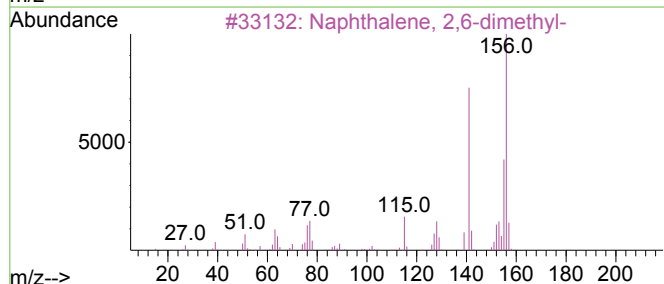
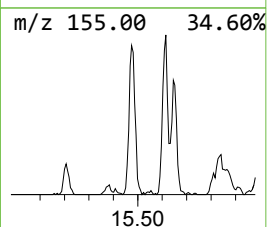
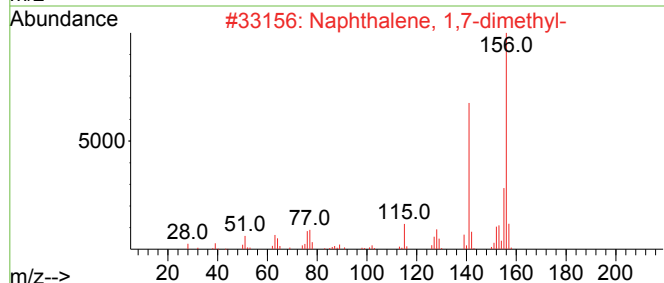
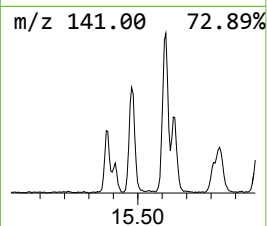
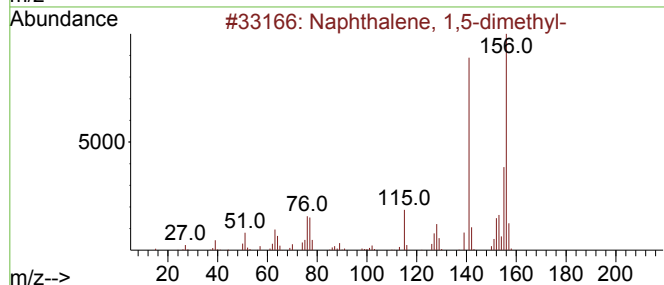
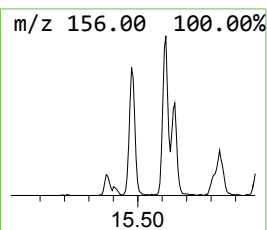
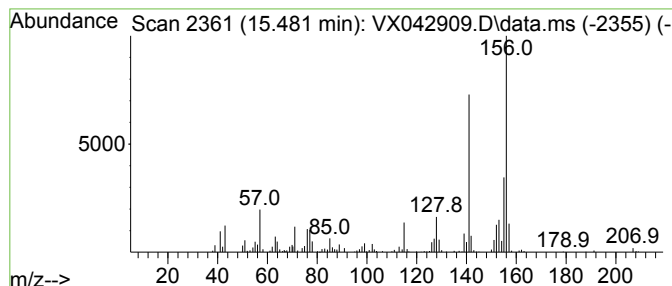
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 1,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	12.73 ug/l	205987	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	98
2			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97



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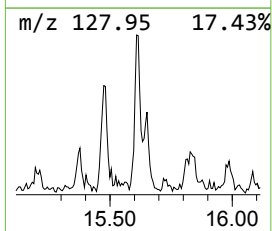
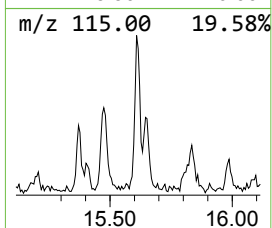
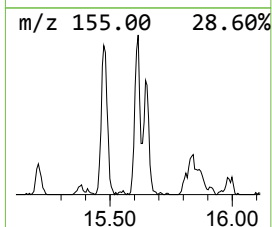
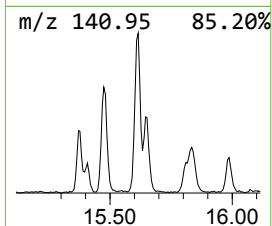
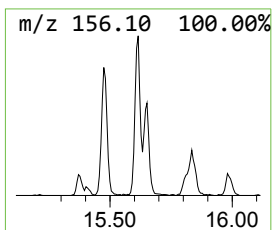
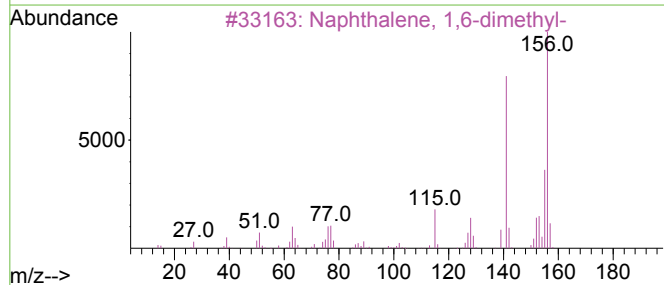
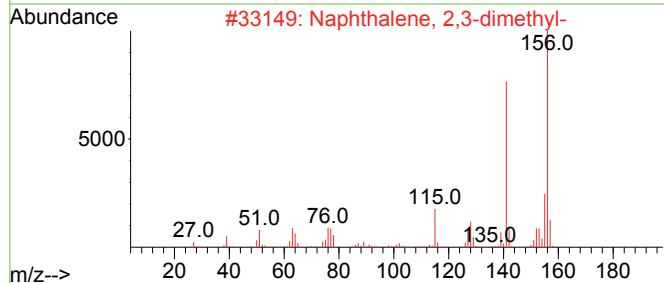
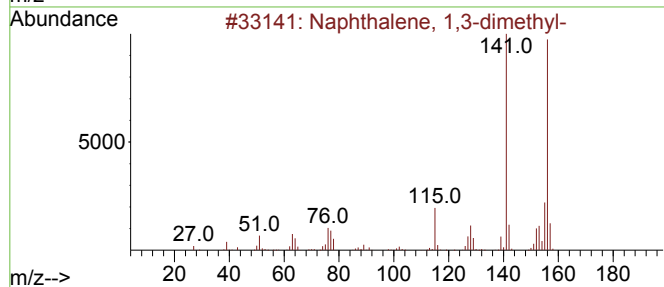
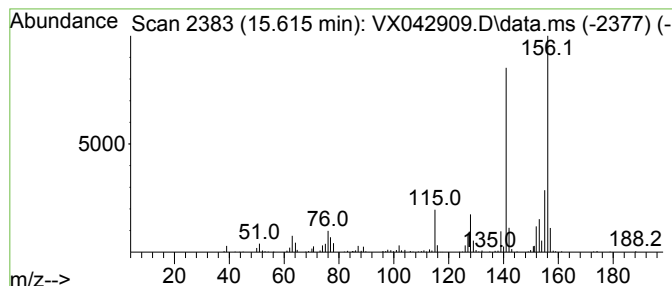
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	12.06 ug/l	195201	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
4			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	95
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042909.D
Acq On : 07 Aug 2024 12:41
Operator : JC/MD
Sample : P3462-05
Misc : 5.04g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-2

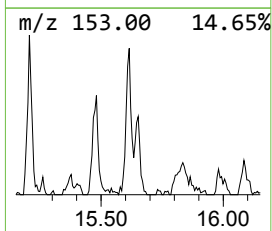
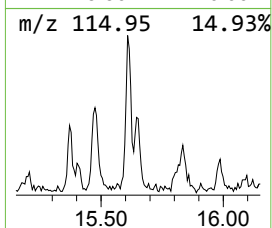
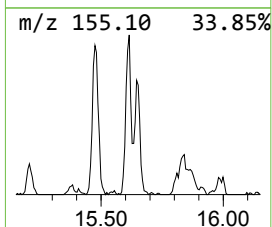
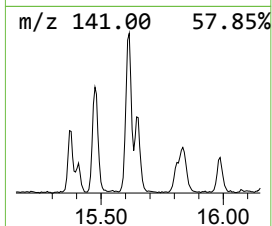
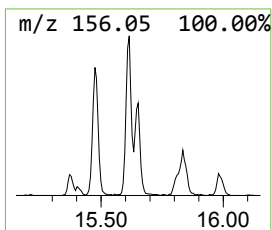
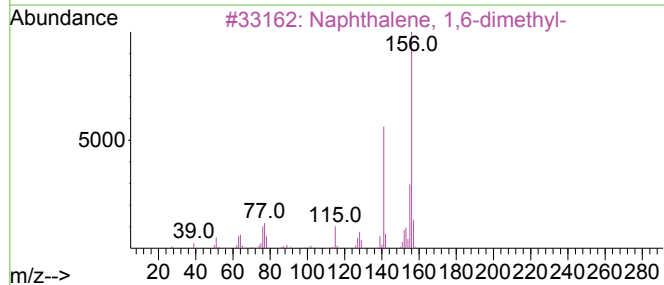
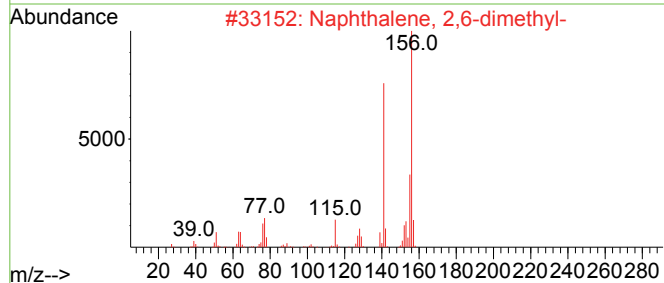
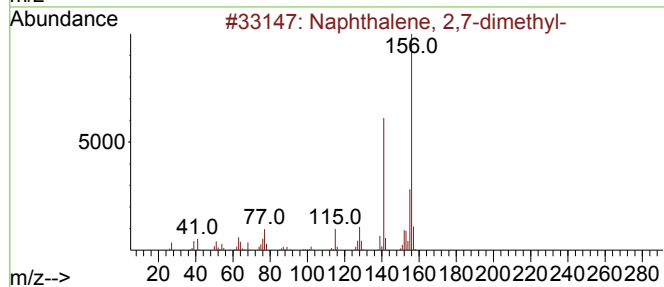
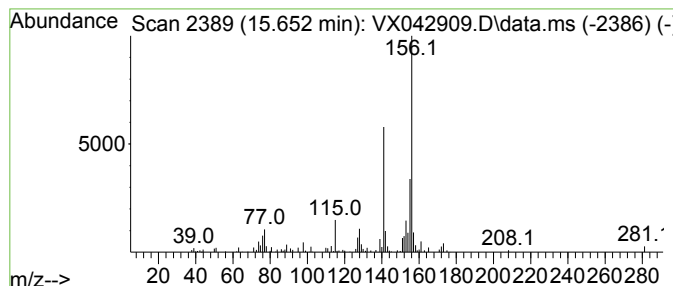
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 2,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.652	6.54 ug/l	105764	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	95
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042909.D
Acq On : 07 Aug 2024 12:41
Operator : JC/MD
Sample : P3462-05
Misc : 5.04g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-2

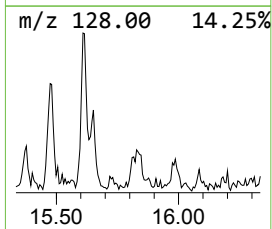
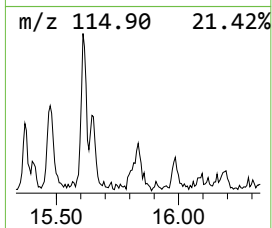
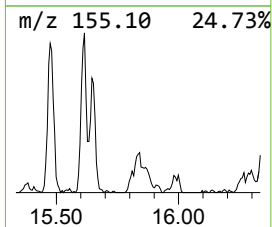
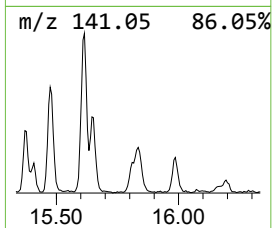
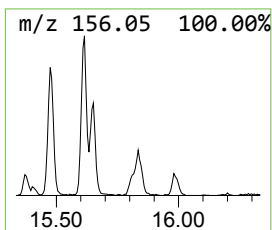
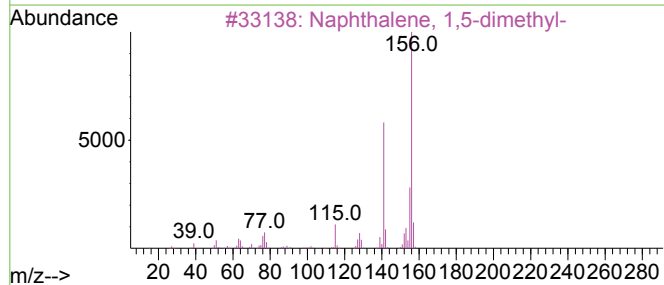
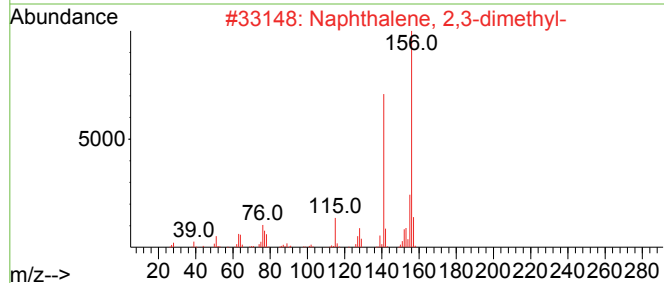
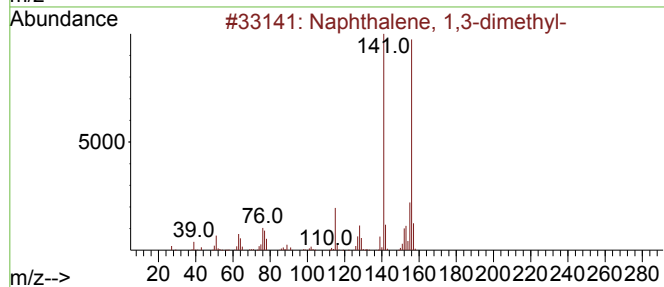
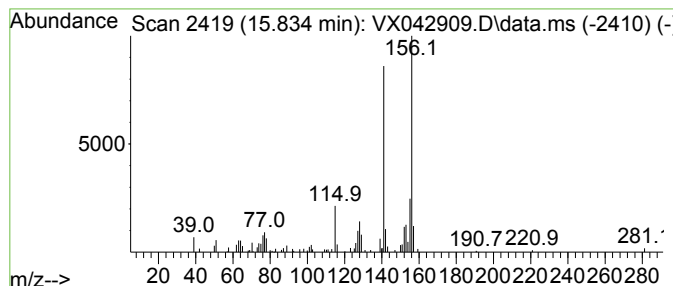
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X080724W.M
Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	5.80 ug/l	93905	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	98
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080724\
Data File : VX042909.D
Acq On : 07 Aug 2024 12:41
Operator : JC/MD
Sample : P3462-05
Misc : 5.04g/10.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
JC-2

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.624	1.624	7.4	ug/l	68604	1	5.550	463365	50.0
Naphthalene, 2-...	14.634	26.0	ug/l	421306	4	12.024	808998	50.0
1H-Indene, 1-et...	14.780	21.2	ug/l	343701	4	12.024	808998	50.0
Naphthalene, 1,...	15.481	12.7	ug/l	205987	4	12.024	808998	50.0
Naphthalene, 1,...	15.615	12.1	ug/l	195201	4	12.024	808998	50.0
Naphthalene, 2,...	15.652	6.5	ug/l	105764	4	12.024	808998	50.0
Naphthalene, 2,...	15.835	5.8	ug/l	93905	4	12.024	808998	50.0