

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
 Data File : VN074472.D
 Acq On : 15 Sep 2022 19:35
 Operator : JC\MD
 Sample : N4553-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 256074-1

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_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074472.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	48	53	60	rBV3	60542	163094	5.11%	0.701%
2	2.634	122	127	130	rBV3	36537	61257	1.92%	0.263%
3	7.234	899	909	918	rBV	84794	230121	7.21%	0.989%
4	7.951	1022	1031	1036	rBV2	365832	857048	26.84%	3.684%
5	8.016	1036	1042	1054	rVB	611111	1367373	42.83%	5.877%
6	8.369	1093	1102	1113	rBV	400664	928884	29.09%	3.992%
7	8.563	1124	1135	1136	rBV4	51570	153655	4.81%	0.660%
8	8.904	1184	1193	1203	rBV	981854	2010402	62.97%	8.641%
9	10.381	1436	1444	1454	rBV	1444446	2617251	81.98%	11.249%
10	11.533	1630	1640	1641	rBV7	14352	32102	1.01%	0.138%
11	11.686	1659	1666	1678	rVB	1541439	2660870	83.34%	11.436%
12	12.674	1823	1834	1846	rBV	1260896	2508387	78.57%	10.781%
13	13.104	1889	1907	1933	rVB3	287380	1757499	55.05%	7.554%
14	13.516	1958	1977	1988	rBV4	596212	2705447	84.74%	11.628%
15	13.616	1988	1994	2016	rVB	1633233	3192716	100.00%	13.722%
16	13.821	2018	2029	2030	rBV9	18325	45318	1.42%	0.195%
17	14.027	2052	2064	2066	rBV4	81345	203067	6.36%	0.873%
18	14.121	2071	2080	2091	rVB4	169637	698549	21.88%	3.002%
19	14.445	2124	2135	2151	rVB3	125087	437731	13.71%	1.881%
20	15.227	2258	2268	2276	rBV5	45098	169234	5.30%	0.727%
21	15.486	2307	2312	2319	rVB10	12754	36089	1.13%	0.155%
22	15.657	2335	2341	2352	rVB7	51500	151647	4.75%	0.652%
23	15.798	2352	2365	2378	rBV6	40026	159655	5.00%	0.686%
24	16.127	2417	2421	2434	rVB10	40386	119341	3.74%	0.513%

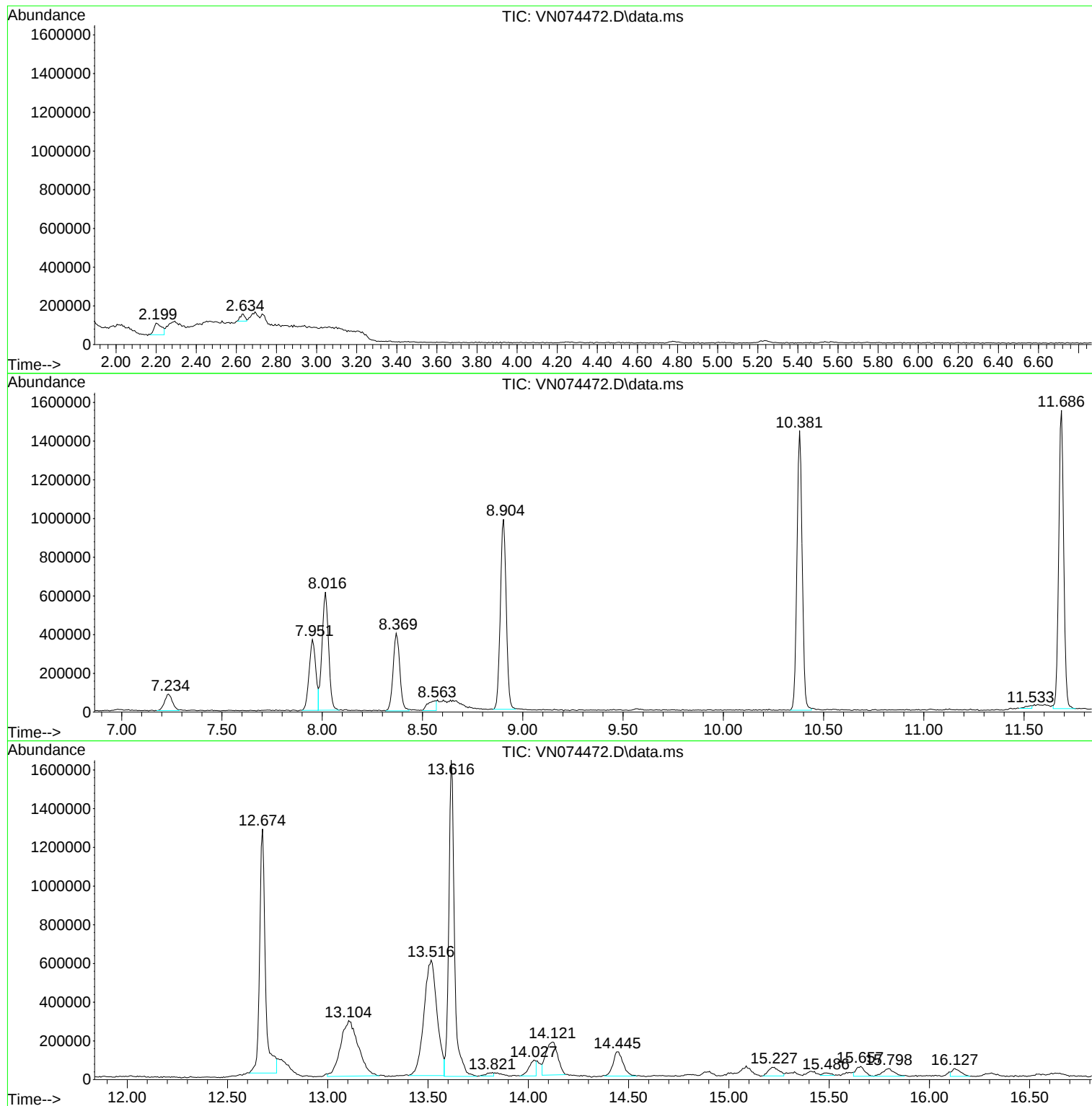
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Quant Title : SW846 8260

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



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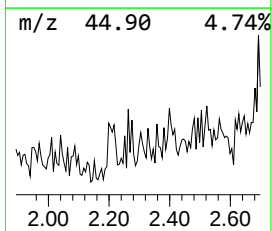
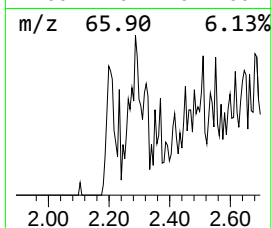
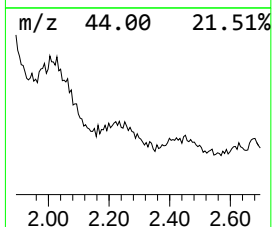
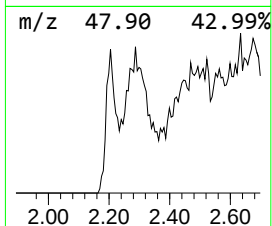
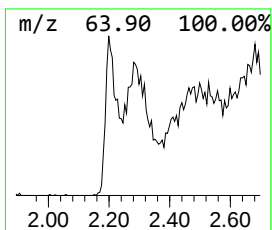
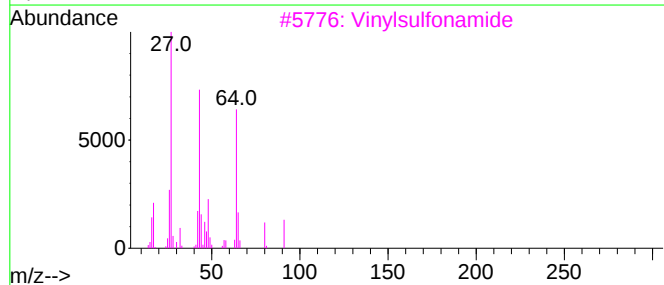
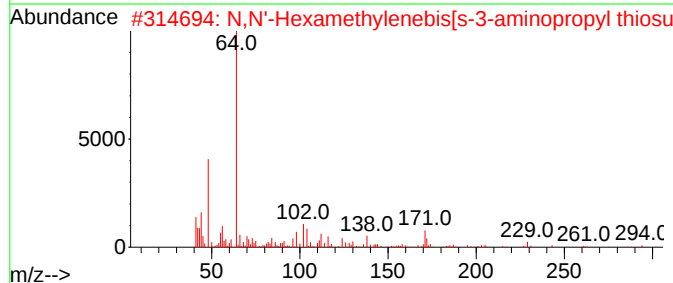
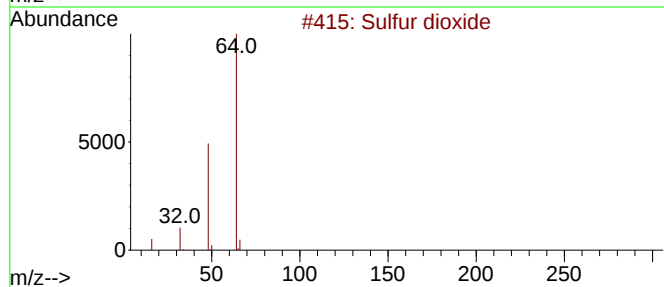
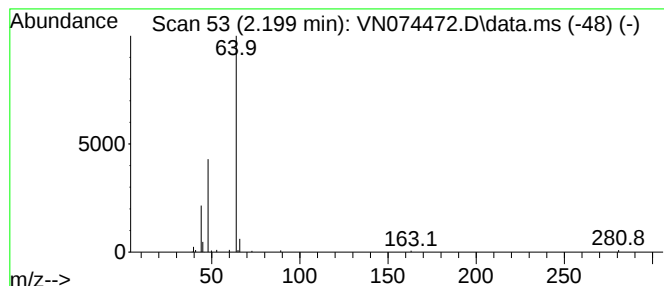
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	5.96 ug/l	163094	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	64
2			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	64
3			Vinylsulfonamide	107	C2H5NO2S	002386-58-5	64
4			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
5			N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	64



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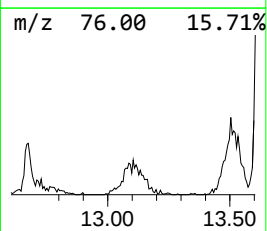
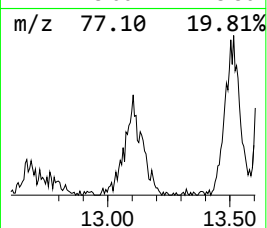
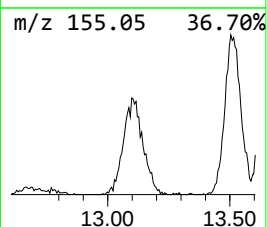
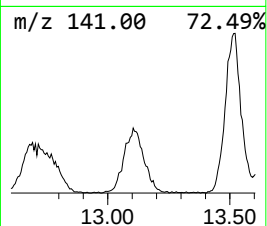
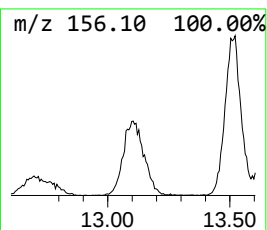
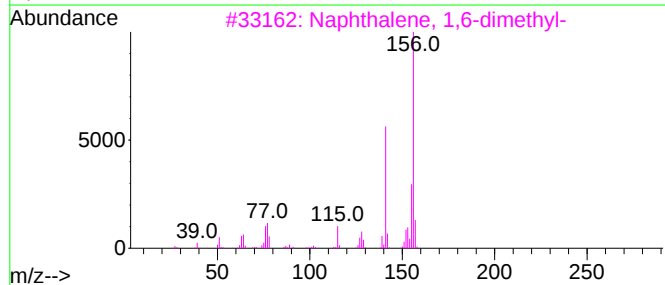
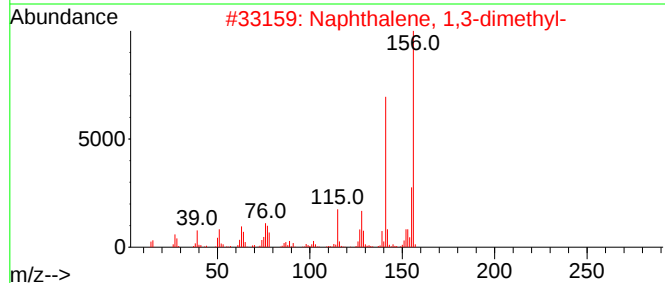
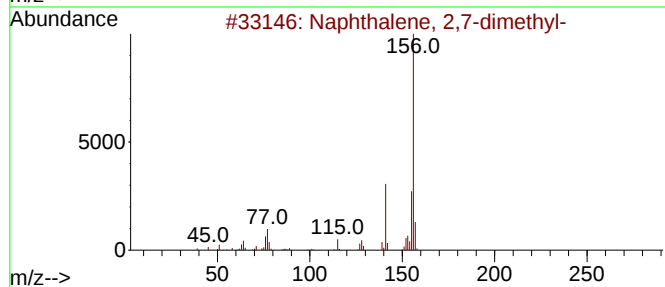
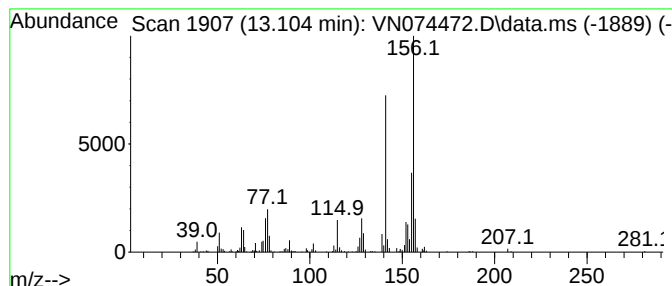
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.104	27.52 ug/l	1757500	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	95
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
5			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93



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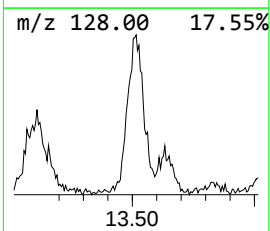
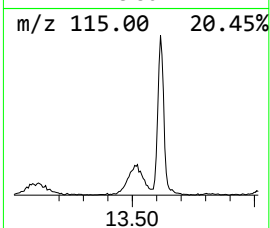
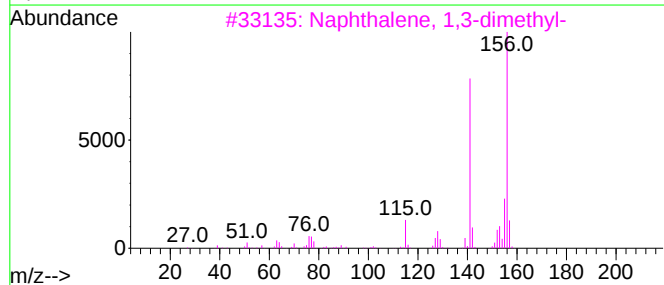
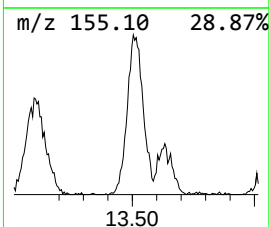
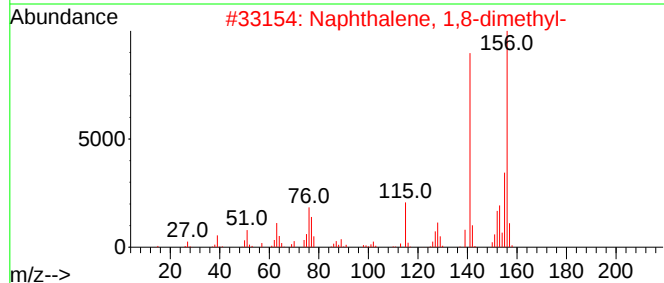
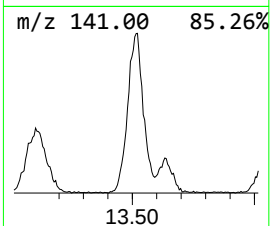
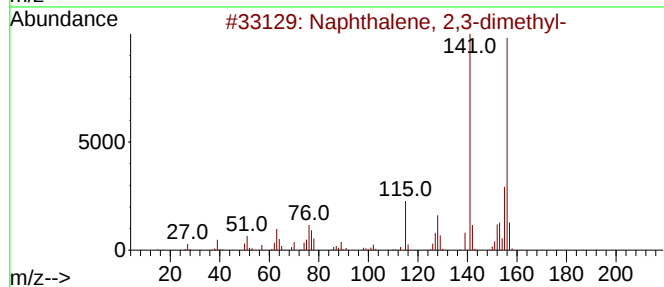
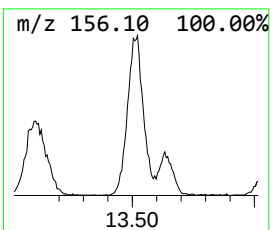
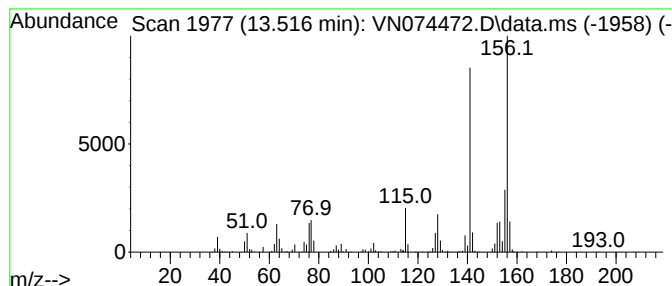
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Quant Title : SW846 8260

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

Peak Number 4 Naphthalene, 2,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.516	42.37 ug/l	2705450	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	98
3			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96



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Instrument :
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ClientSampleId :
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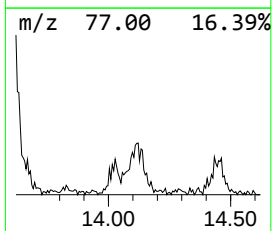
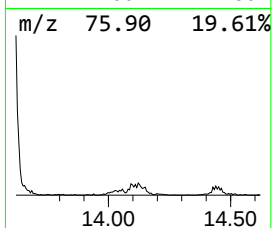
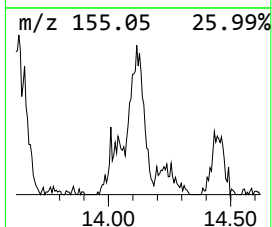
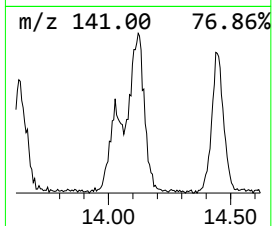
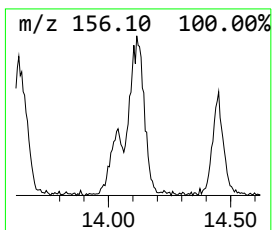
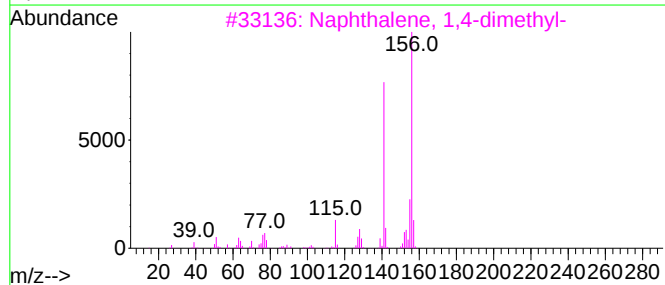
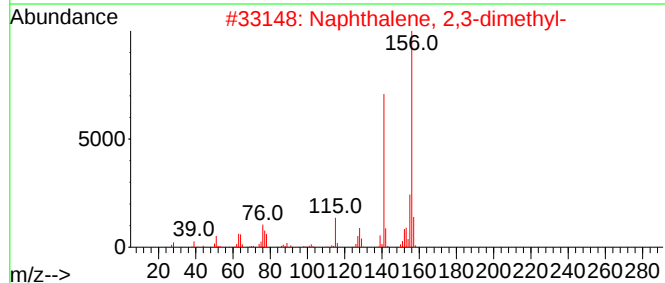
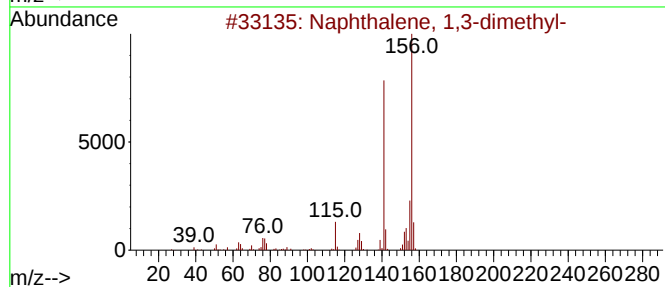
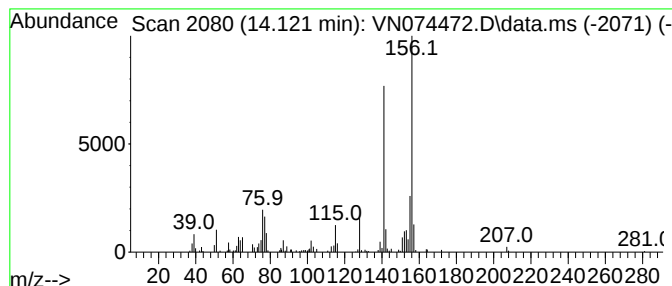
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.121	10.94 ug/l	698549	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	93
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	93
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	93
4			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	91



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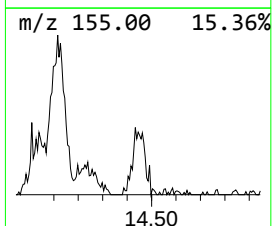
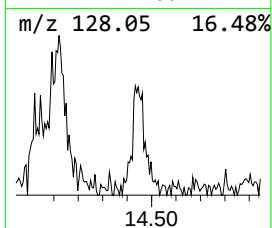
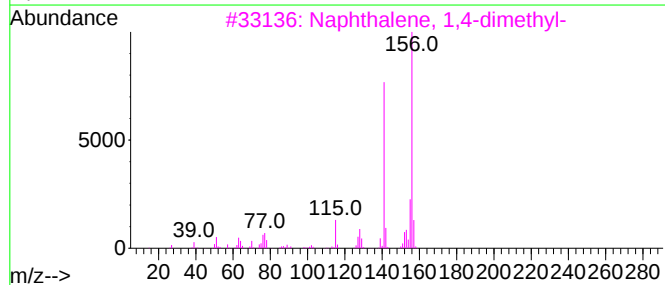
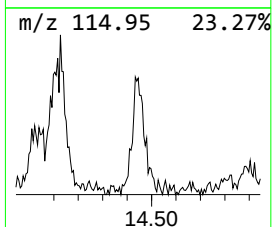
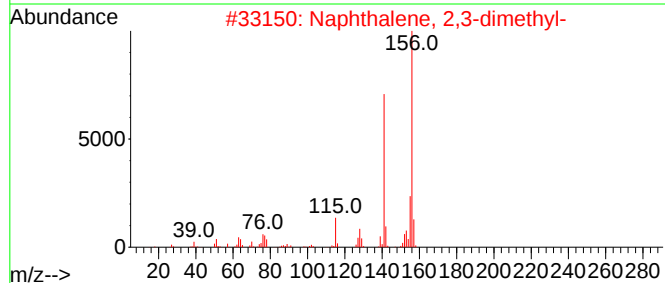
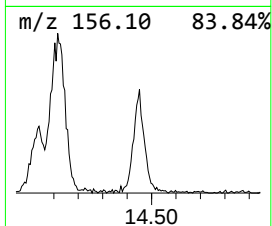
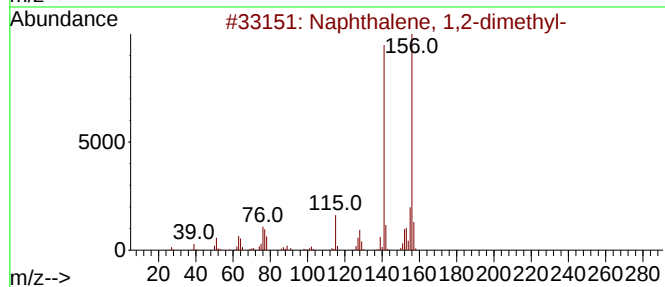
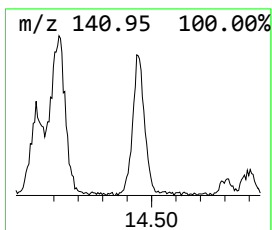
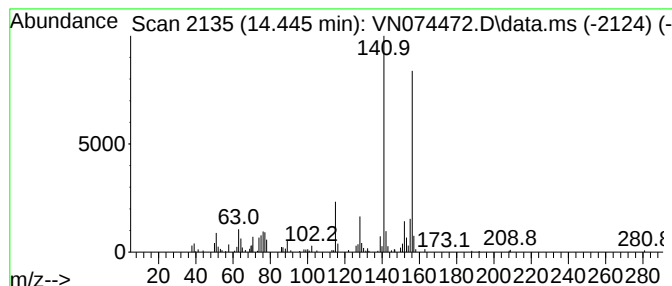
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Quant Title : SW846 8260

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

Peak Number 6 Naphthalene, 1,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	6.86 ug/l	437731	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2-dimethyl-	156	C12H12	000573-98-8	92
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	91
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	91
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	87
5			Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	6.0	ug/l	163094	1	8.016	1367370	50.0
Naphthalene, 2,...	13.104	27.5	ug/l	1757500	4	13.616	3192720	50.0
Naphthalene, 2,...	13.516	42.4	ug/l	2705450	4	13.616	3192720	50.0
Naphthalene, 1,...	14.121	10.9	ug/l	698549	4	13.616	3192720	50.0
Naphthalene, 1,...	14.445	6.9	ug/l	437731	4	13.616	3192720	50.0