

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013122\
 Data File : VN070856.D
 Acq On : 31 Jan 2022 16:59
 Operator : JC/MD
 Sample : N1284-01
 Misc : 3.47g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 S-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\82N011822W.M
 Title : SW846 8260

Signal : TIC: VN070856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.231	77	90	102	rBV4	38143	96325	2.14%	0.344%
2	4.851	1047	1067	1104	rBV2	44609	152027	3.37%	0.543%
3	8.016	2224	2247	2258	rBV	504996	1215352	26.96%	4.344%
4	8.078	2258	2270	2305	rVB	1072056	2509290	55.65%	8.969%
5	8.432	2376	2402	2435	rBV	638278	1487977	33.00%	5.318%
6	8.963	2580	2600	2631	rBV	1525286	3233488	71.72%	11.557%
7	10.438	3132	3150	3190	rBV	2359224	4508658	100.00%	16.115%
8	11.049	3364	3378	3391	rBV3	37648	62714	1.39%	0.224%
9	11.341	3477	3487	3500	rVB5	34466	60068	1.33%	0.215%
10	11.451	3517	3528	3537	rBV4	36881	58889	1.31%	0.210%
11	11.548	3557	3564	3579	rVB5	26325	48744	1.08%	0.174%
12	11.744	3617	3637	3659	rBV	2117390	3929181	87.15%	14.043%
13	11.937	3695	3709	3718	rBV8	41300	90738	2.01%	0.324%
14	11.985	3719	3727	3736	rVV4	47305	77202	1.71%	0.276%
15	12.181	3792	3800	3810	rVB4	41100	60641	1.34%	0.217%
16	12.251	3811	3826	3838	rBV8	110654	284497	6.31%	1.017%
17	12.366	3858	3869	3880	rVB	458882	722113	16.02%	2.581%
18	12.452	3881	3901	3902	rBV4	167756	281334	6.24%	1.006%
19	12.731	3989	4005	4021	rVB	1728194	3034465	67.30%	10.846%
20	12.975	4082	4096	4106	rBV9	144647	339381	7.53%	1.213%
21	13.053	4110	4125	4138	rBV9	333218	932278	20.68%	3.332%
22	13.195	4171	4178	4187	rVB3	123807	159808	3.54%	0.571%
23	13.533	4297	4304	4308	rBV3	164761	225909	5.01%	0.807%
24	13.672	4344	4356	4368	rBV	1884382	3225593	71.54%	11.529%
25	13.997	4468	4477	4486	rBV4	327726	529707	11.75%	1.893%
26	14.506	4657	4667	4680	rVB5	408490	652429	14.47%	2.332%

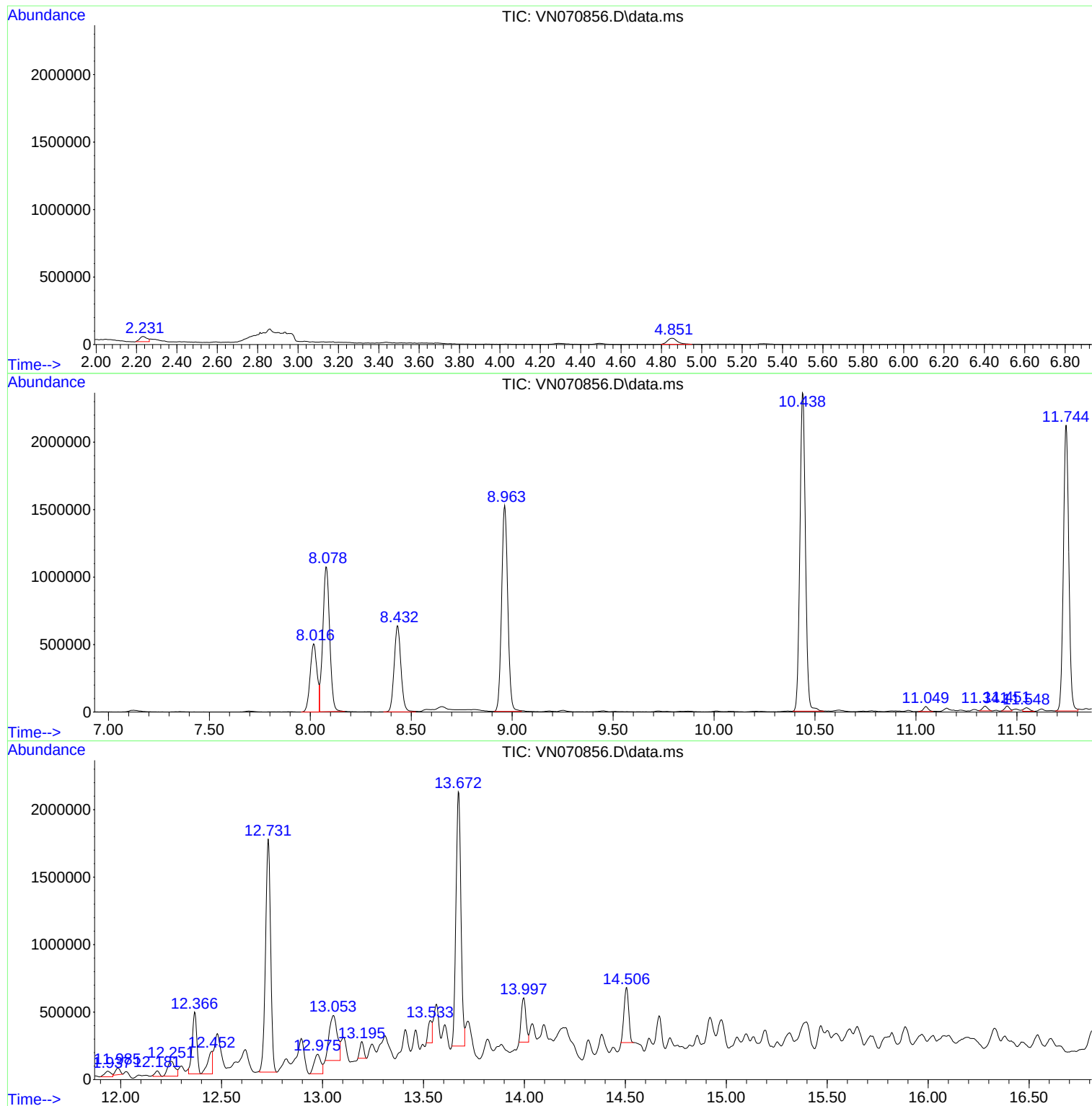
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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



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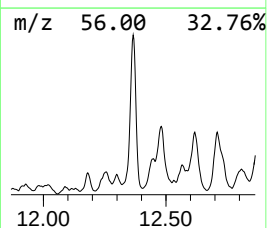
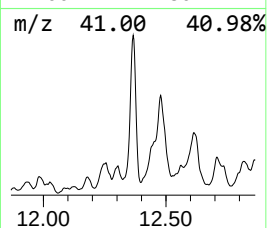
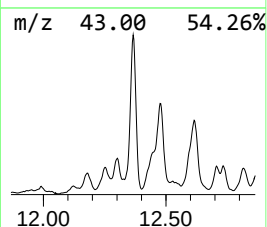
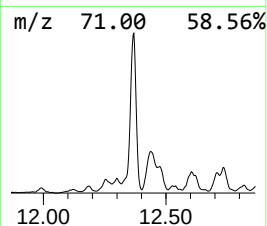
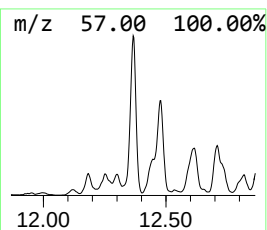
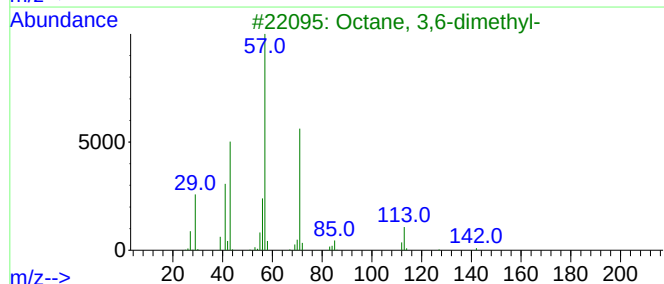
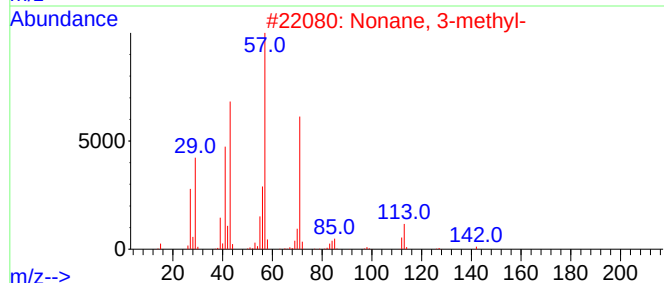
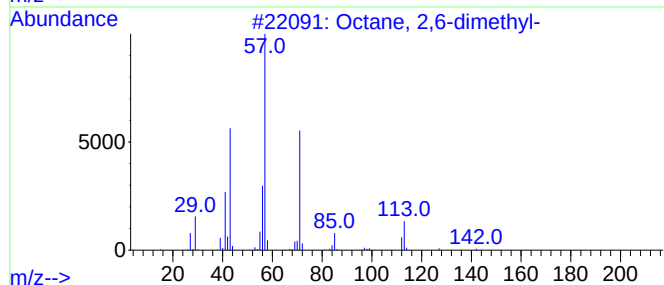
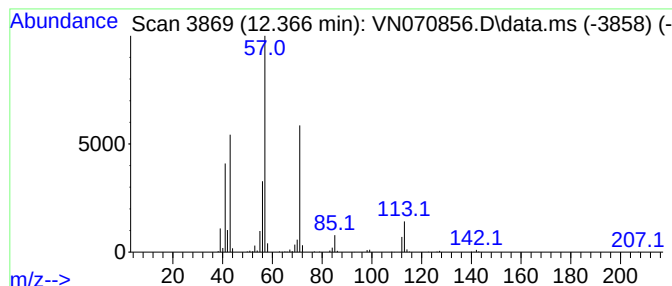
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011822W.M
Quant Title : SW846 8260

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

Peak Number 1 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.366	9.19 ug/l	722113	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	93
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	91
3			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	90
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	64
5			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	64



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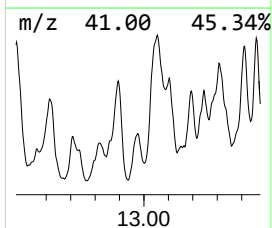
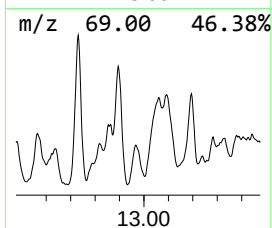
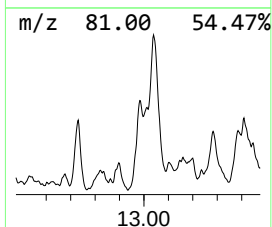
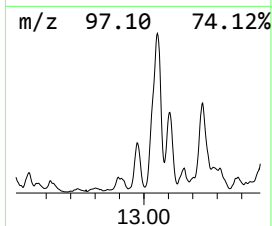
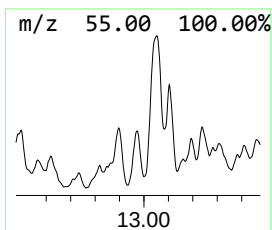
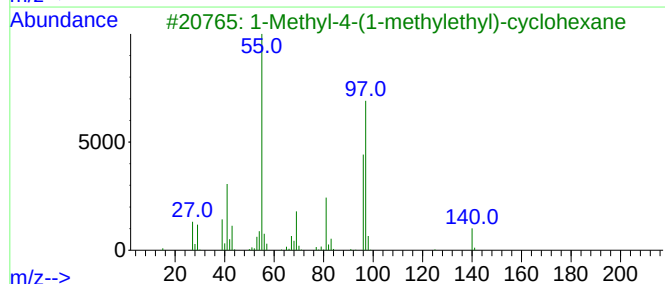
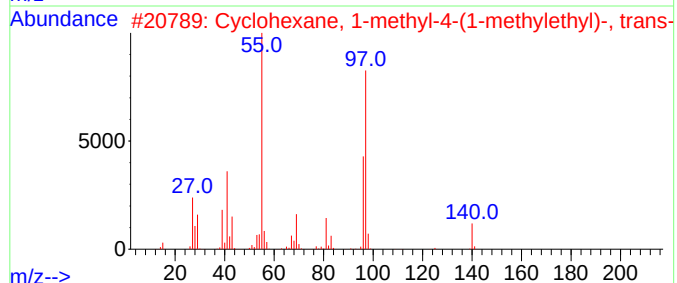
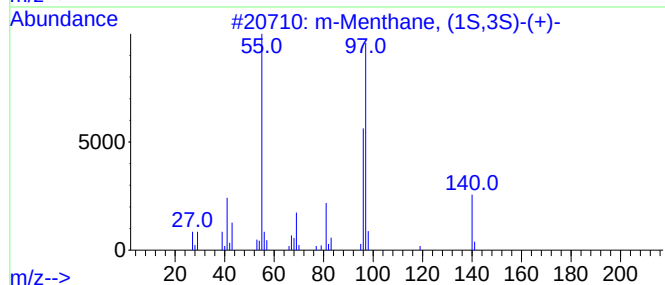
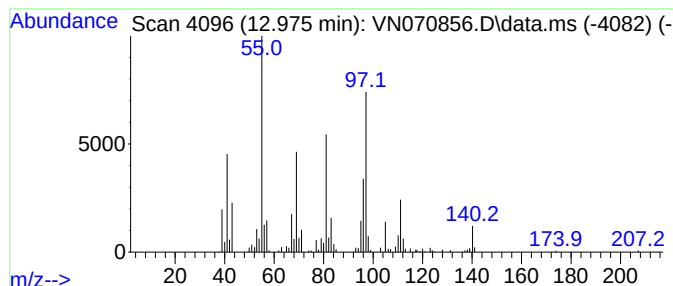
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Peak Number 2 m-Menthane, (1S,3S)-(+)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	5.26 ug/l	339381	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	64
2			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	62
3			1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	58
4			Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	58
5			Cyclohexane, 1-methyl-3-propyl-	140	C10H20	004291-80-9	52



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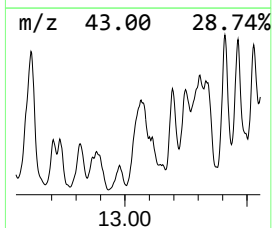
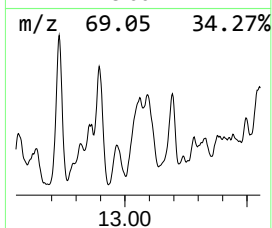
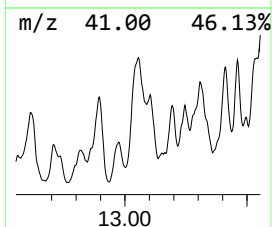
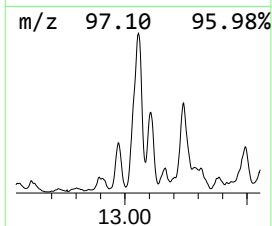
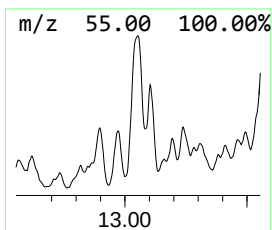
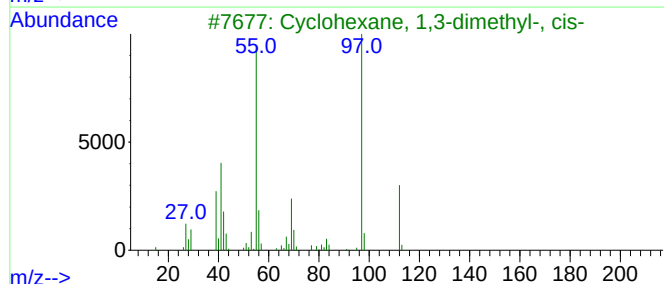
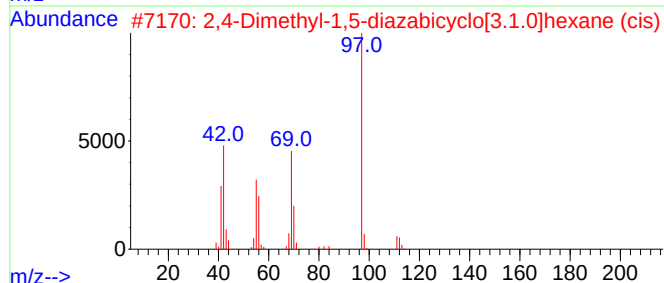
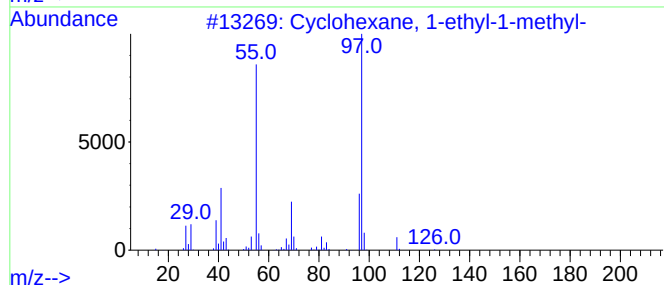
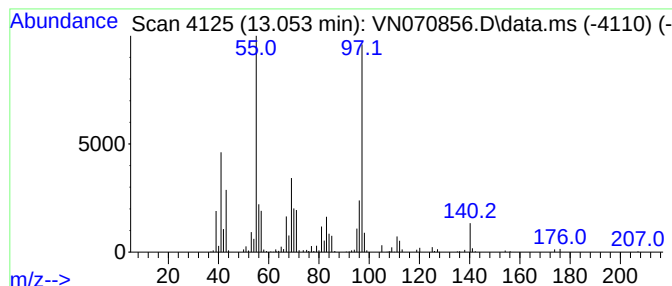
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexane, 1-ethyl-1-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.053	14.45 ug/l	932278	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	52
2			2,4-Dimethyl-1,5-diazabicyclo[3...]	112	C6H12N2	100463-01-2	52
3			Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	52
4			2,4-Dimethyl-1,5-diazabicyclo[3...]	112	C6H12N2	1000283-20-9	52
5			Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	52



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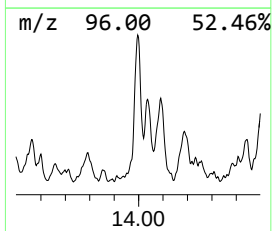
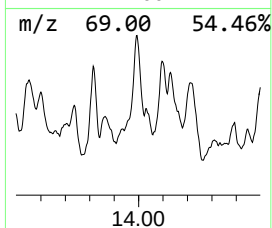
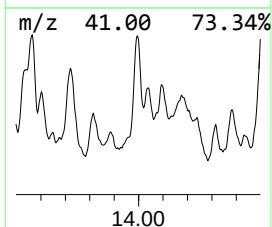
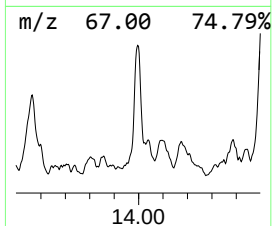
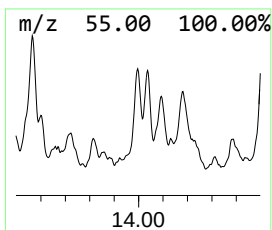
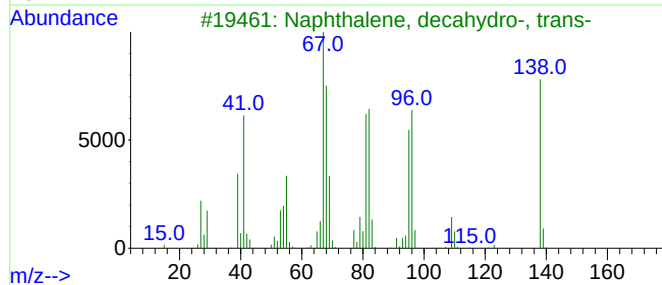
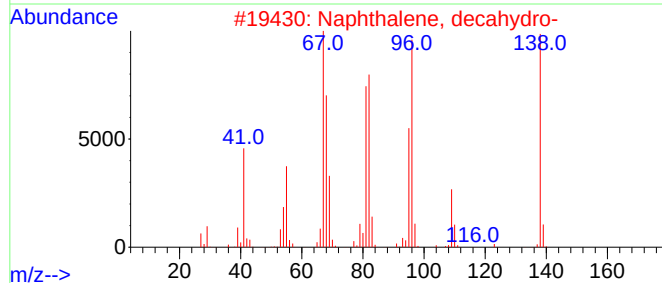
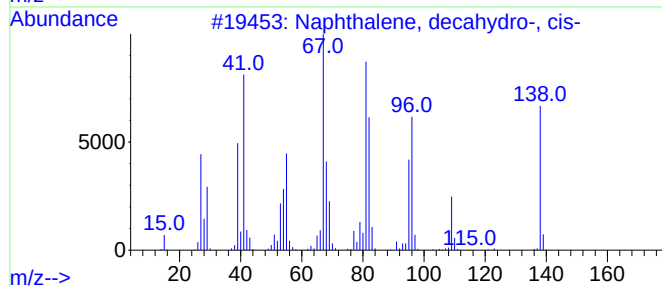
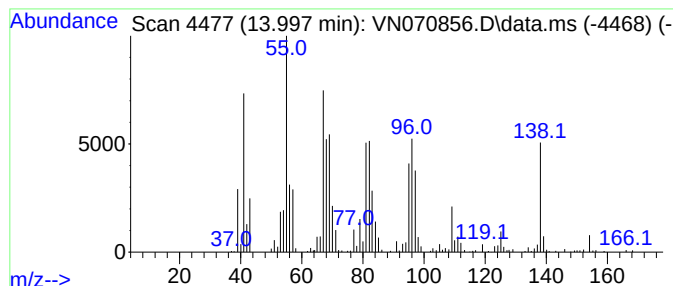
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, decahydro-, cis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	8.21 ug/l	529707	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	96
2			Naphthalene, decahydro-	138	C10H18	000091-17-8	96
3			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	94
4			Spiro[4.5]decane	138	C10H18	000176-63-6	90
5			9-Borabicyclo[3.3.1]nonane, 9-hy...	138	C8H15BO	063366-65-4	87



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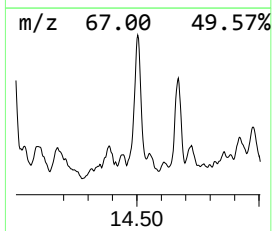
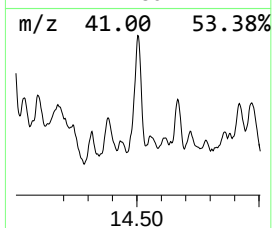
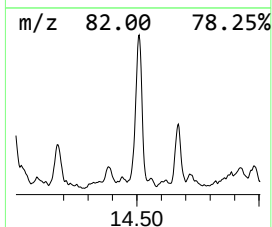
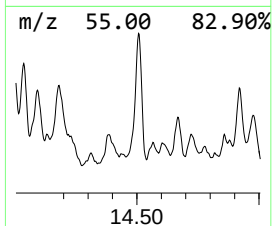
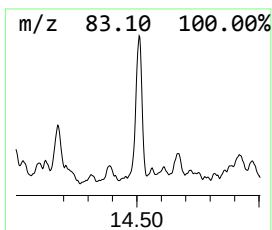
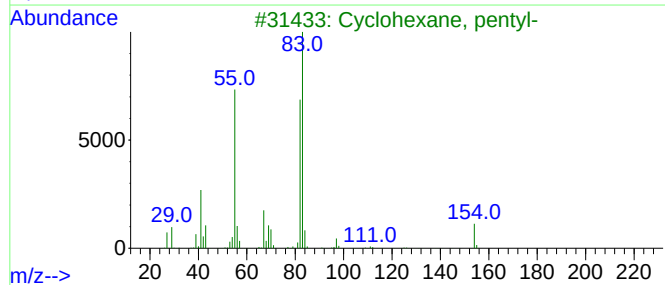
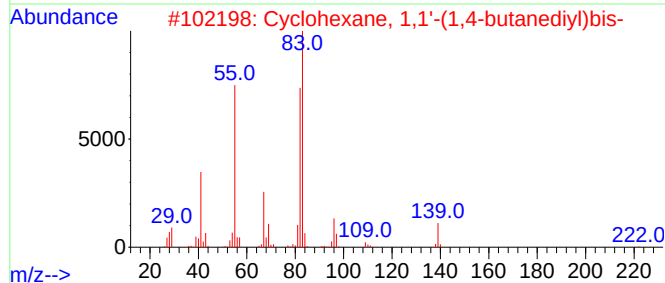
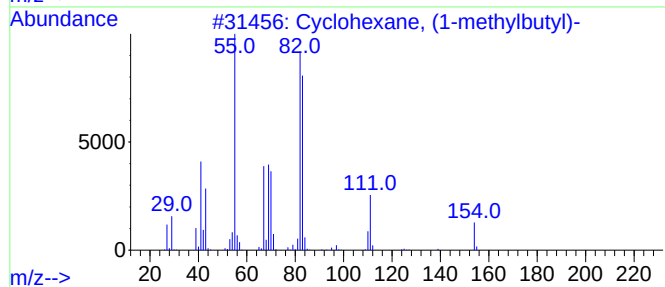
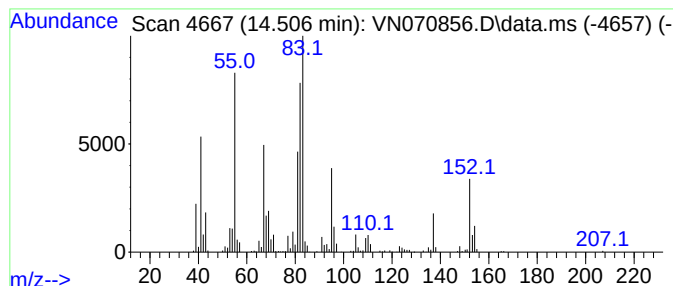
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Quant Title : SW846 8260

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

Peak Number 5 Cyclohexane, (1-methylbutyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.506	10.11 ug/l	652429	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (1-methylbutyl)-	154	C11H22	061208-94-4	58
2			Cyclohexane, 1,1'-(1,4-butanediyl)-	222	C16H30	006165-44-2	50
3			Cyclohexane, pentyl-	154	C11H22	004292-92-6	49
4			(Z)-(Z)-Hex-3-en-1-yl 2-methylbu...	182	C11H18O2	084060-80-0	43
5			(E)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	120603-00-1	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Octane, 2,6-dim...	12.366	9.2	ug/l	722113	3	11.744	3929180	50.0
m-Menthane, (1S...	12.975	5.3	ug/l	339381	4	13.672	3225590	50.0
Cyclohexane, 1-...	13.053	14.4	ug/l	932278	4	13.672	3225590	50.0
Naphthalene, de...	13.997	8.2	ug/l	529707	4	13.672	3225590	50.0
Cyclohexane, (1...	14.506	10.1	ug/l	652429	4	13.672	3225590	50.0