

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
 Data File : VN085855.D
 Acq On : 25 Feb 2025 14:24
 Operator : JC\MD
 Sample : Q1395-01
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 BEL-25-0005

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\82N021825W.M
 Title : SW846 8260

Signal : TIC: VN085855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.159	1045	1055	1059	rBV	192665	459806	7.17%	1.346%
2	8.212	1059	1064	1074	rVV2	547853	1265694	19.73%	3.706%
3	8.318	1074	1082	1093	rVB3	84260	212161	3.31%	0.621%
4	8.436	1093	1102	1111	rBV	355120	798667	12.45%	2.338%
5	8.571	1117	1125	1135	rVB	197480	440434	6.87%	1.289%
6	8.700	1135	1147	1155	rBV4	45004	134130	2.09%	0.393%
7	8.959	1182	1191	1202	rVV	220856	433273	6.75%	1.268%
8	9.094	1205	1214	1232	rVB	473452	990836	15.45%	2.901%
9	9.594	1287	1299	1310	rBV6	31359	91442	1.43%	0.268%
10	10.565	1455	1464	1468	rBV	705098	1256084	19.58%	3.677%
11	10.630	1468	1475	1488	rVB	3490968	6414249	100.00%	18.779%
12	11.865	1676	1685	1697	rBV	597091	1075988	16.77%	3.150%
13	12.065	1712	1719	1724	rBV2	53815	119256	1.86%	0.349%
14	12.376	1762	1772	1782	rBV6	52596	192112	3.00%	0.562%
15	12.835	1840	1850	1859	rBV2	710458	1776194	27.69%	5.200%
16	12.929	1859	1866	1876	rBV9	25653	96626	1.51%	0.283%
17	13.018	1876	1881	1887	rVB3	79178	160543	2.50%	0.470%
18	13.094	1887	1894	1897	rBV3	93425	184643	2.88%	0.541%
19	13.171	1902	1907	1913	rVB7	69931	157060	2.45%	0.460%
20	13.488	1956	1961	1965	rBV3	77654	160750	2.51%	0.471%
21	13.535	1965	1969	1978	rVB2	152831	328674	5.12%	0.962%
22	13.618	1978	1983	1986	rBV3	81245	155033	2.42%	0.454%
23	13.671	1987	1992	1998	rVB4	126755	285813	4.46%	0.837%
24	13.788	2006	2012	2021	rVB	653663	1247766	19.45%	3.653%
25	13.870	2021	2026	2030	rBV4	159988	316064	4.93%	0.925%
26	13.976	2041	2044	2048	rBV3	106030	166607	2.60%	0.488%
27	14.118	2062	2068	2080	rBV5	505718	1120692	17.47%	3.281%
28	14.223	2080	2086	2095	rBV9	159227	598333	9.33%	1.752%
29	14.329	2100	2104	2115	rVB8	234239	523274	8.16%	1.532%
30	14.435	2117	2122	2127	rBV2	263119	498049	7.76%	1.458%
31	14.506	2130	2134	2139	rVB5	234843	374747	5.84%	1.097%
32	14.570	2140	2145	2149	rBV5	277481	486602	7.59%	1.425%
33	14.623	2149	2154	2159	rBV	919516	1572443	24.51%	4.604%
34	14.729	2169	2172	2175	rBV4	139333	215637	3.36%	0.631%
35	14.794	2178	2183	2187	rVV	742382	1278864	19.94%	3.744%
36	14.841	2187	2191	2198	rVB4	567590	1089166	16.98%	3.189%

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Title : SW846 8260

37	15.106	2231	2236	2244	rVB4	962763	1817281	28.33%	5.320%
38	15.223	2251	2256	2259	rBV3	819459	1494505	23.30%	4.375%
39	15.312	2267	2271	2278	rVB5	632301	1201435	18.73%	3.517%
40	15.670	2327	2332	2338	rBV5	1058974	2965997	46.24%	8.683%

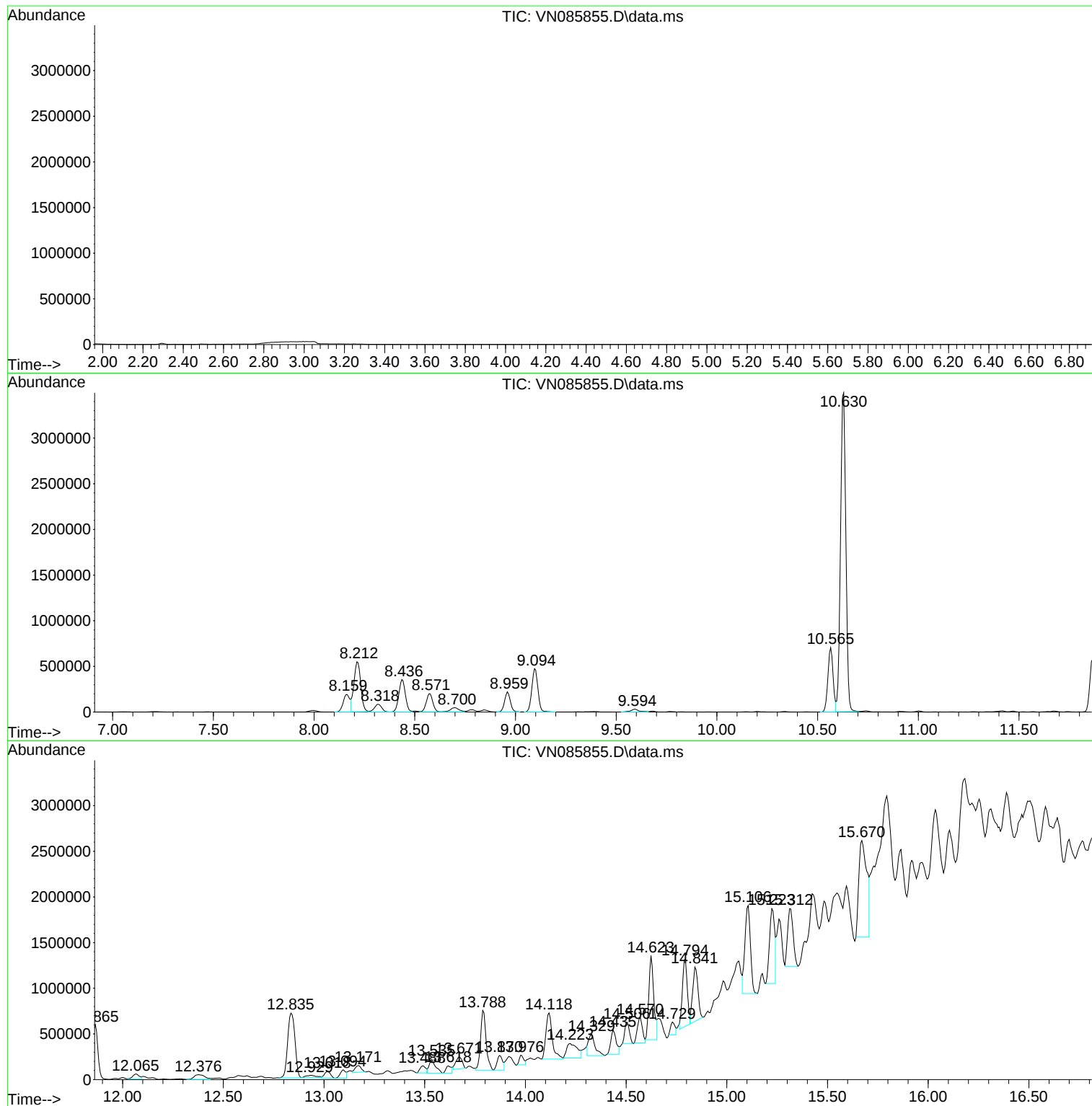
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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



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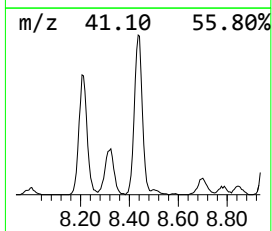
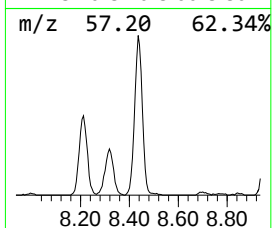
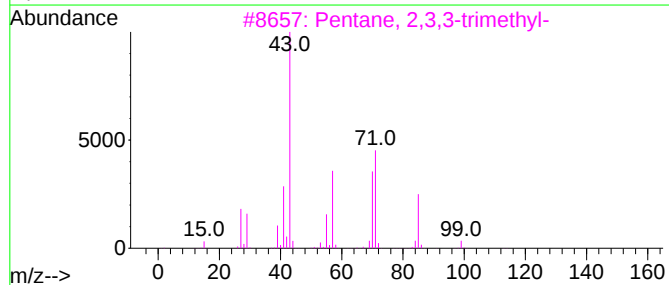
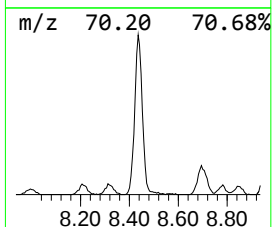
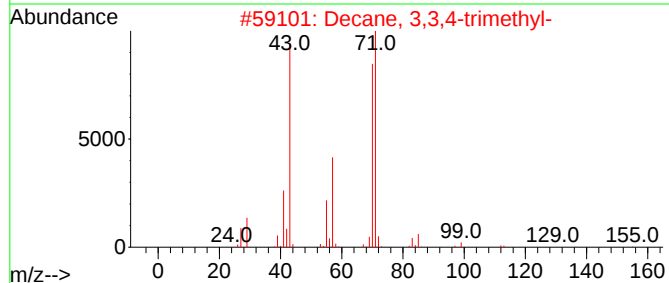
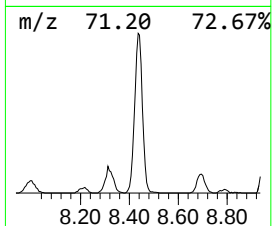
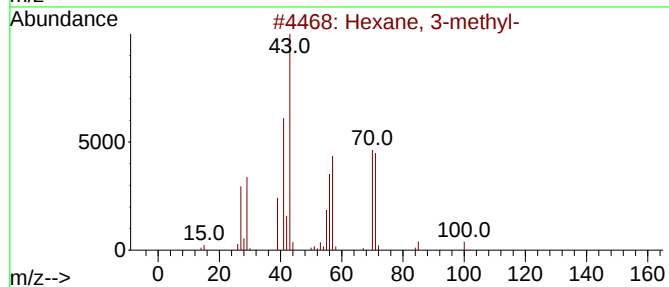
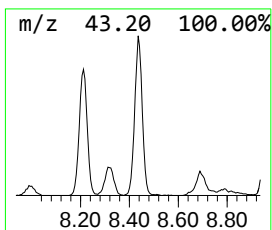
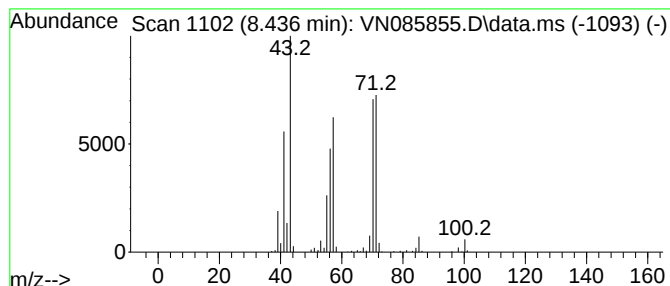
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.436	31.55 ug/l	798667	Pentafluorobenzene	8.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	58
3			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	53
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	53



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Instrument :
MSVOA_N
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BEL-25-0005

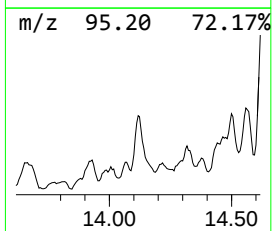
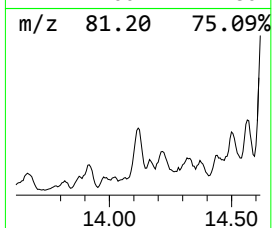
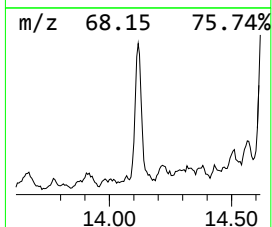
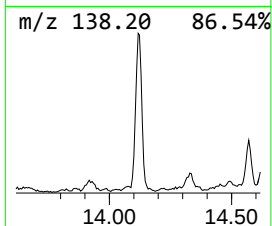
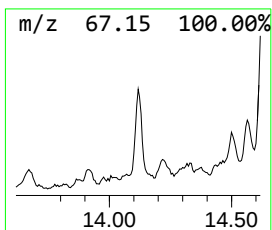
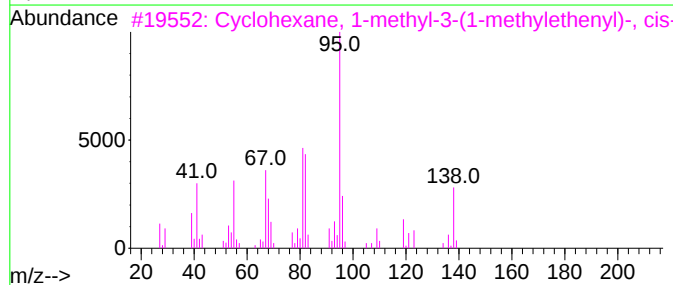
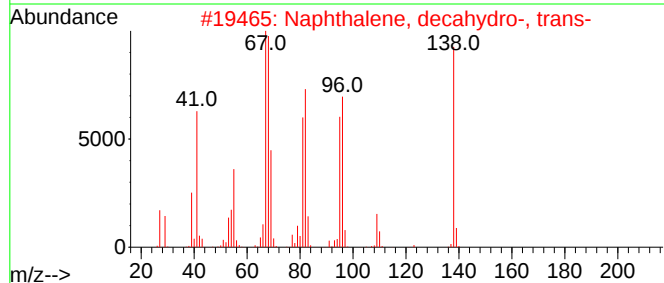
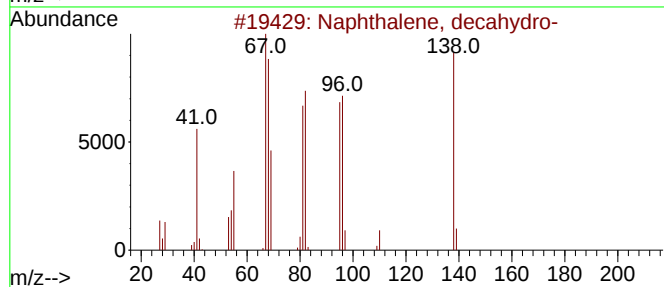
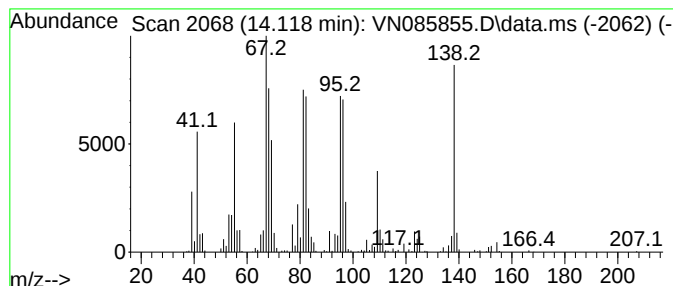
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, decahydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.118	44.91 ug/l	1120690	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-	138	C10H18	000091-17-8	97
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	94
3			Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	91
4			Spiro[4.5]decane	138	C10H18	000176-63-6	89
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	83



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ALS Vial : 11 Sample Multiplier: 1

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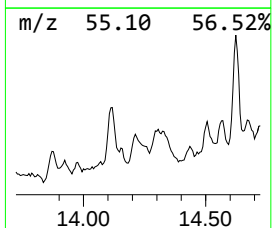
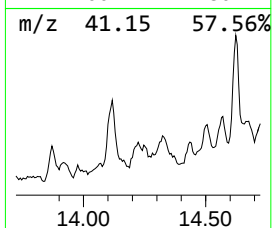
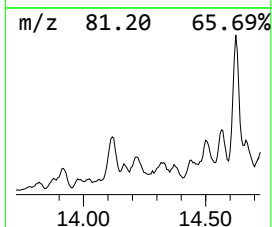
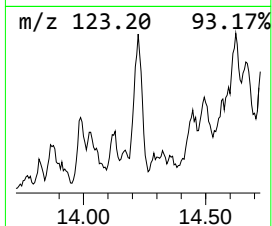
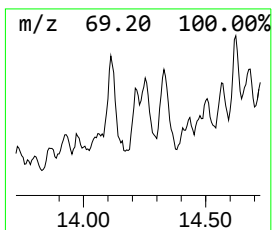
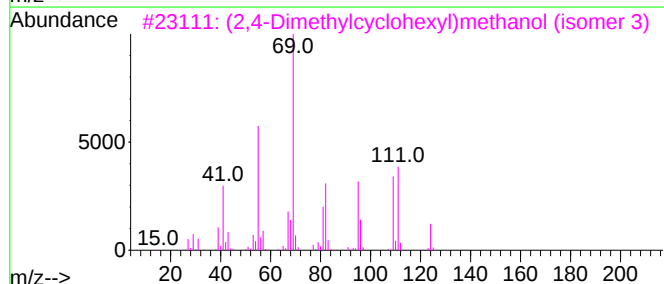
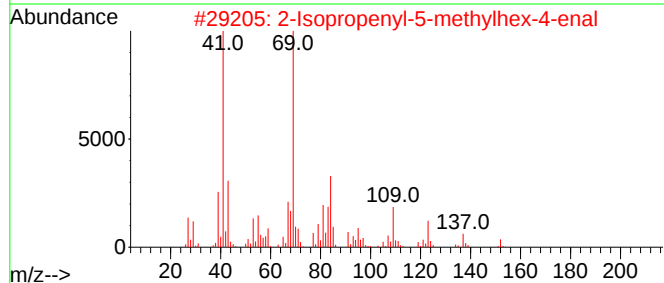
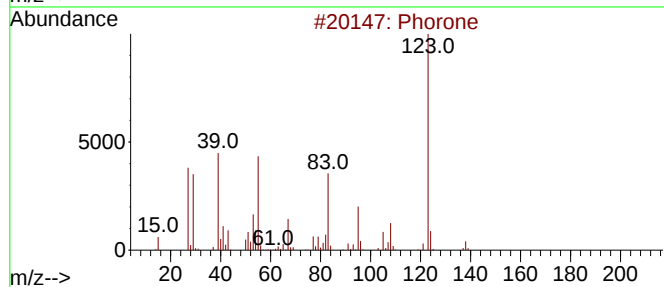
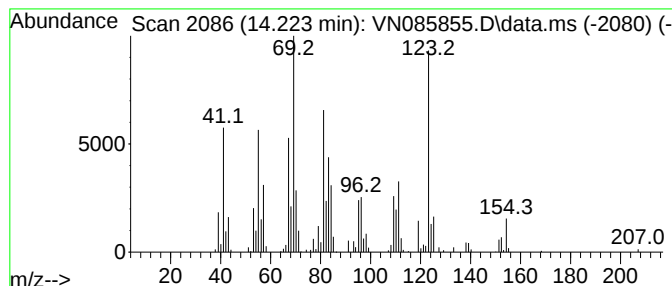
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown14.223 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.223	23.98 ug/l	598333	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phorone	138	C9H14O	000504-20-1	38
2			2-Isopropenyl-5-methylhex-4-enal	152	C10H16O	075697-98-2	38
3			(2,4-Dimethylcyclohexyl)methanol...	142	C9H18O	1000499-02-8	35
4			Cyclopentane, hexyl-	154	C11H22	004457-00-5	30
5			Neral	152	C10H16O	000106-26-3	30



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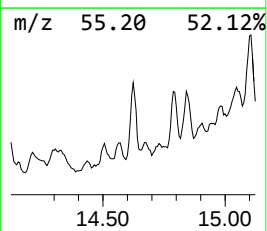
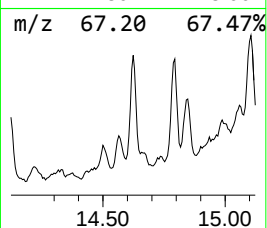
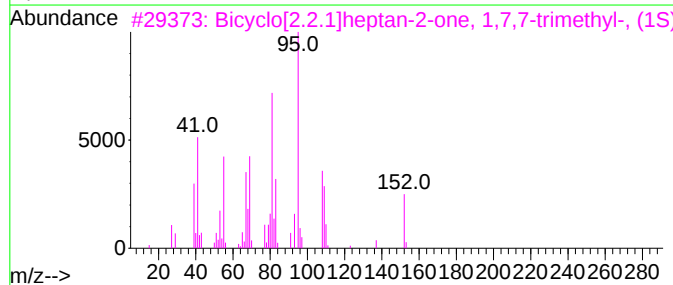
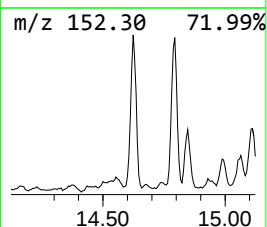
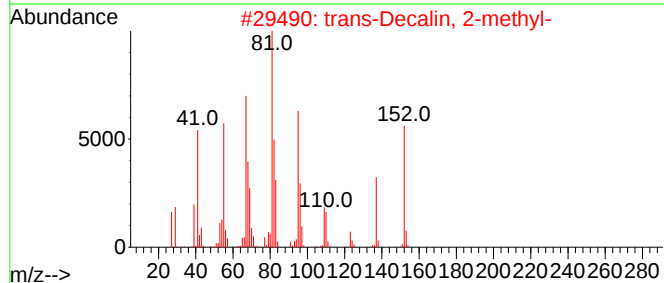
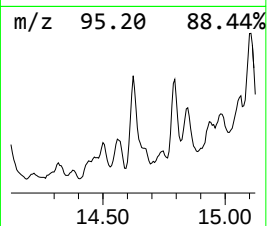
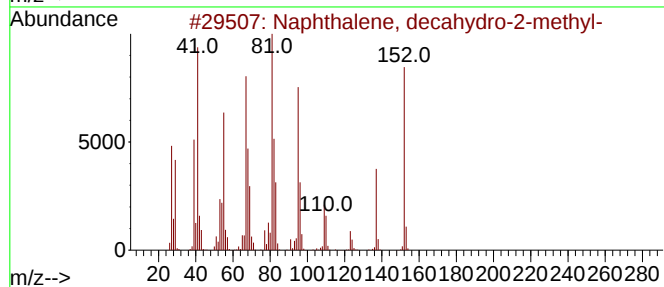
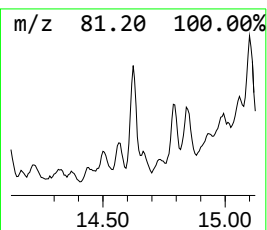
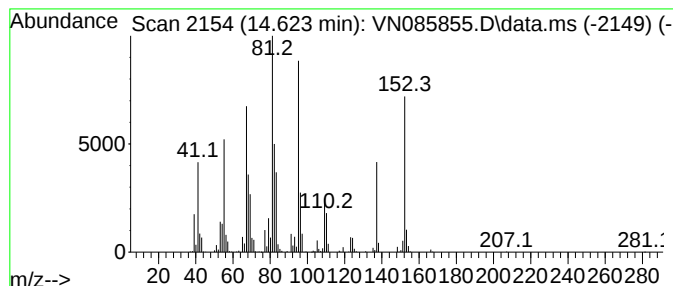
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Peak Number 4 Naphthalene, decahydro-2-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.623	63.01 ug/l	1572440	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	97
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	93
3			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	68
4			Pulegone	152	C10H16O	000089-82-7	58
5			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	58



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BEL-25-0005

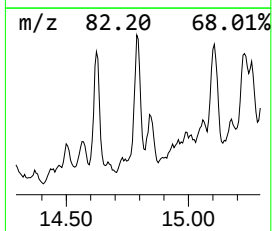
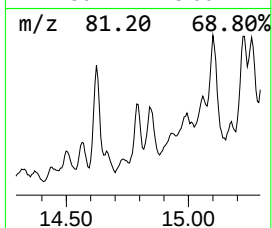
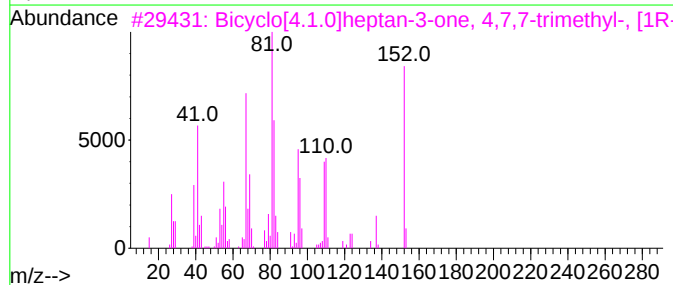
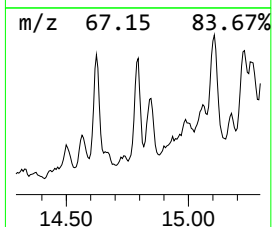
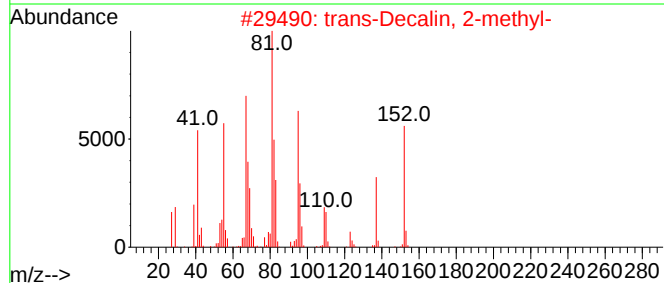
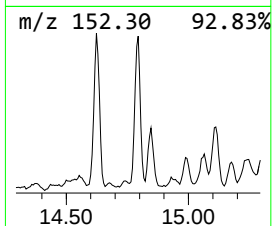
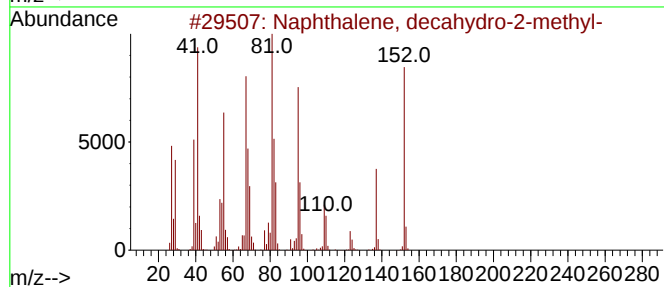
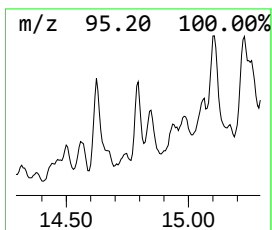
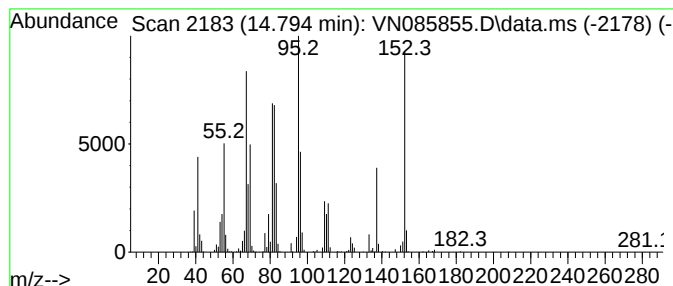
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Quant Title : SW846 8260

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

Peak Number 5 trans-Decalin, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.794	51.25 ug/l	1278860	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	87
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	86
3			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	58
4			Pulegone	152	C10H16O	000089-82-7	58
5			Bicyclo[2.2.1]heptane, 1,3,3-tri...	138	C10H18	006248-88-0	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

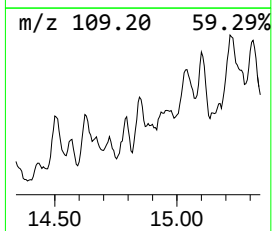
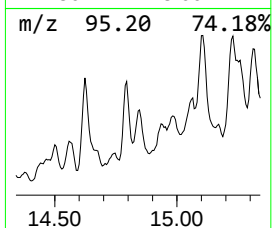
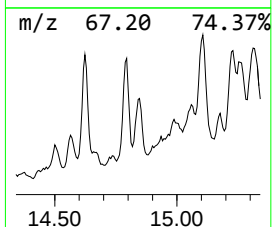
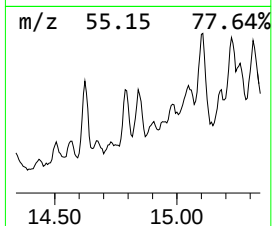
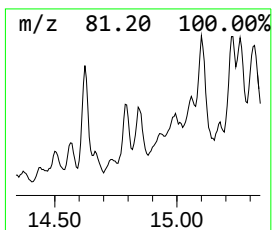
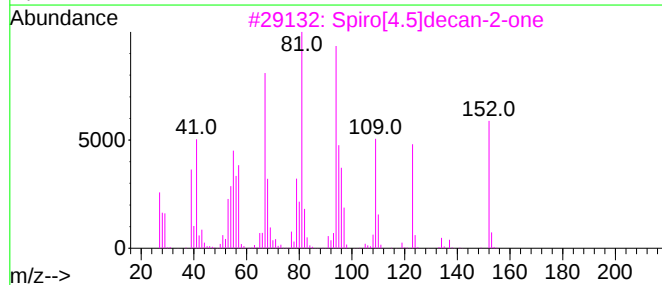
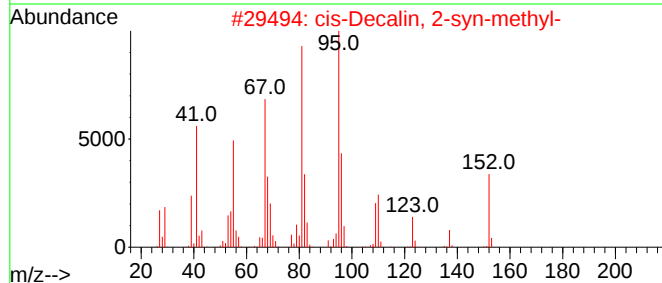
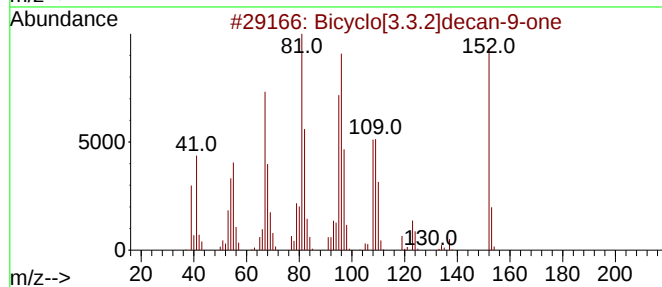
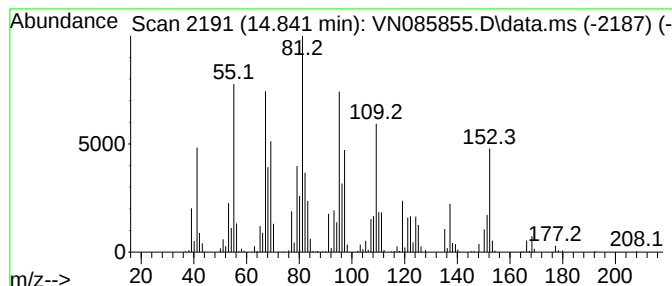
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Quant Title : SW846 8260

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

Peak Number 6 Bicyclo[3.3.2]decan-9-one Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.841	43.64 ug/l	1089170	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	72
2			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	70
3			Spiro[4.5]decan-2-one	152	C10H16O	003643-16-1	68
4			2(1H)-Naphthalenone, octahydro-,...	152	C10H16O	016021-08-2	64
5			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

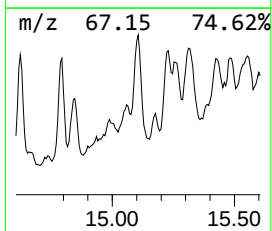
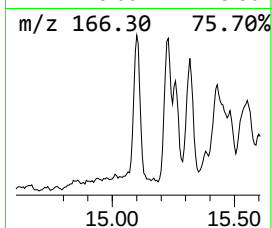
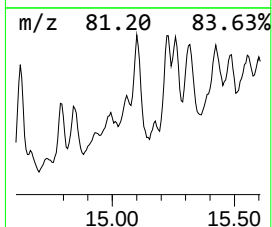
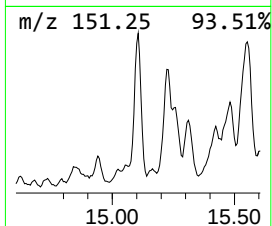
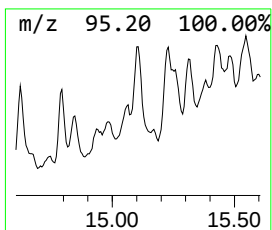
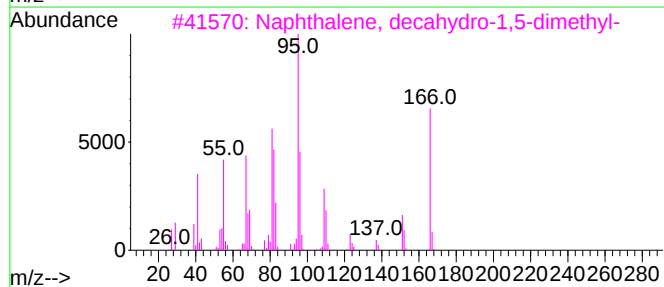
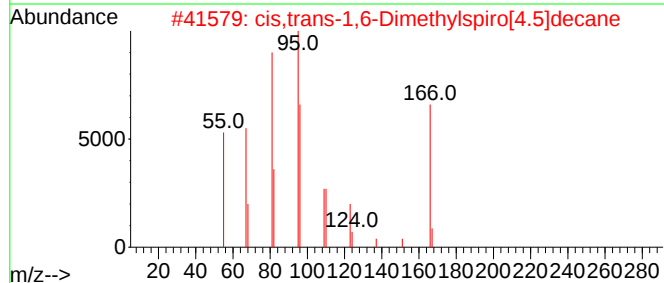
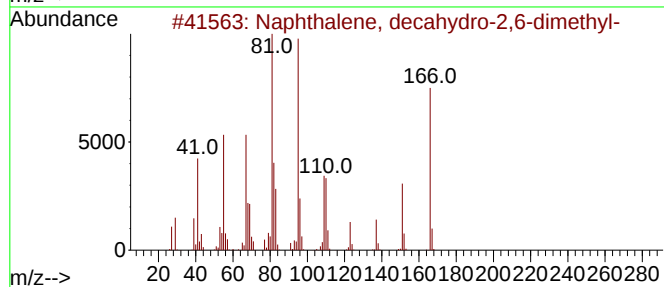
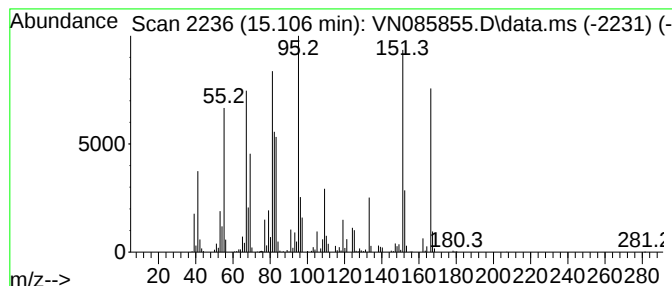
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Quant Title : SW846 8260

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

Peak Number 7 Naphthalene, decahydro-2,6-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.106	72.82 ug/l	1817280	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	62
2			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	58
3			Naphthalene, decahydro-1,5-dimet...	166	C12H22	066552-62-3	58
4			cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	53
5			trans,trans-1,6-Dimethylspiro[4...	166	C12H22	1000111-72-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

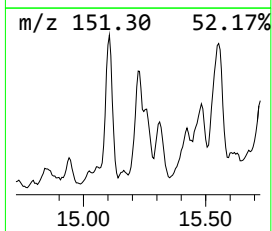
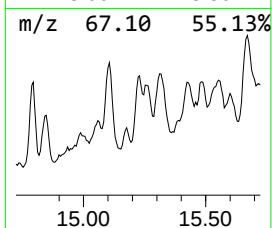
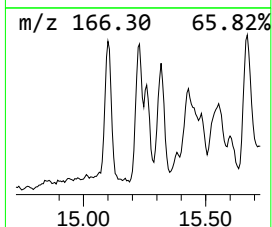
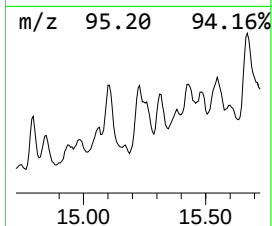
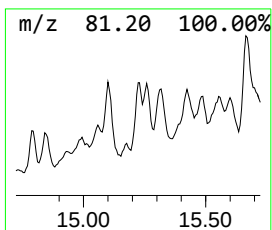
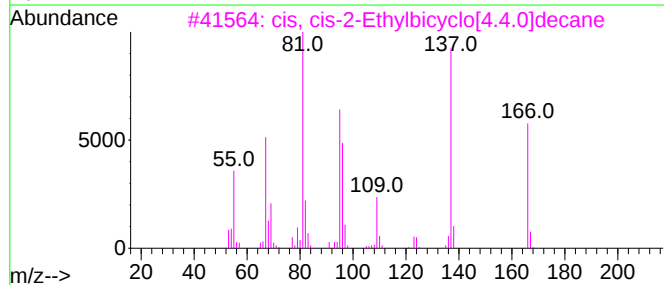
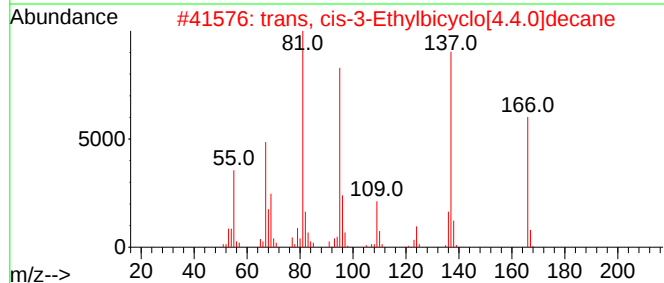
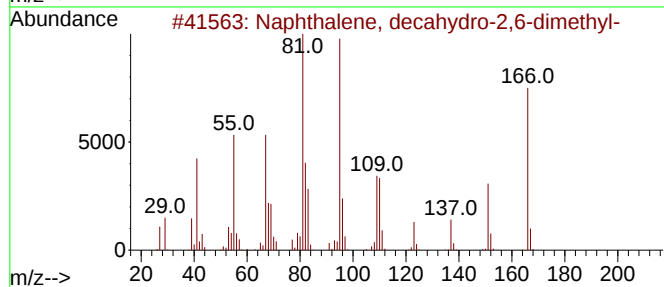
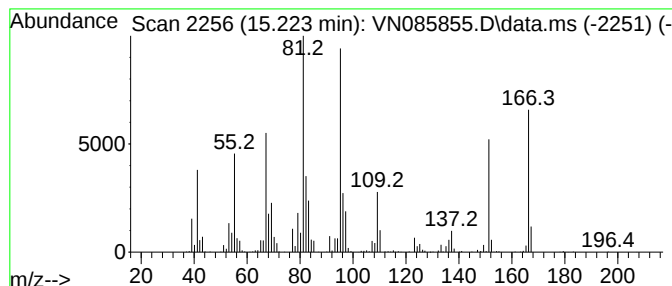
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Quant Title : SW846 8260

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

Peak Number 8 trans, cis-3-Ethylbicyclo[4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.223	59.89 ug/l	1494510	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	91
2			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	87
3			cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	74
4			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	72
5			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

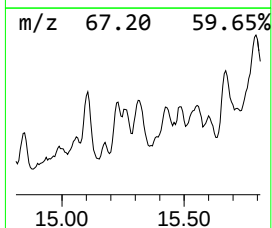
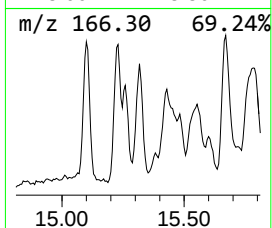
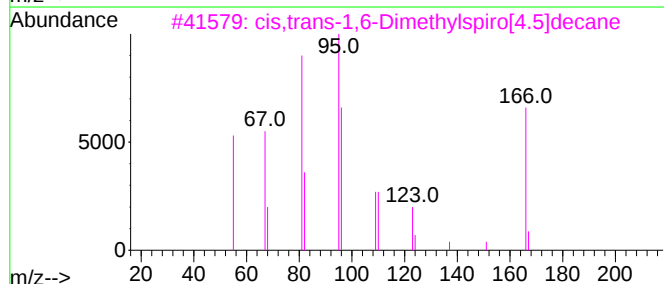
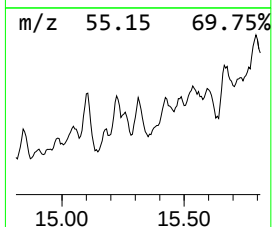
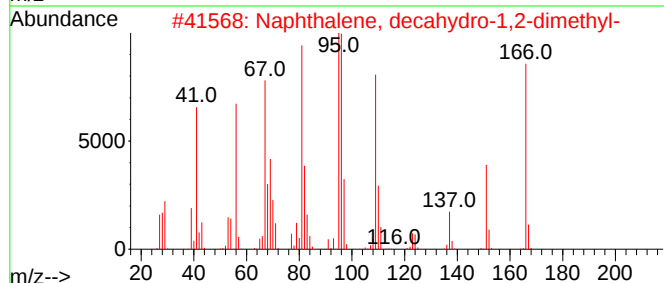
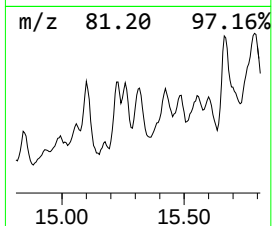
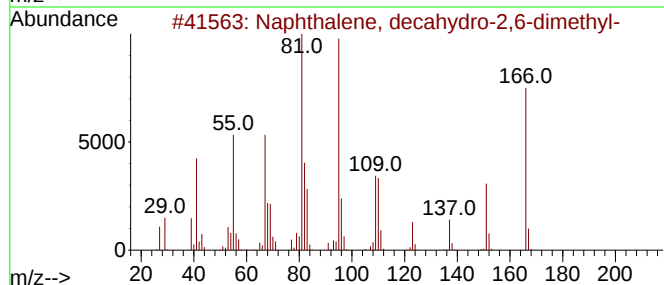
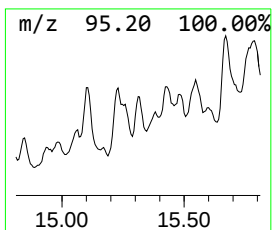
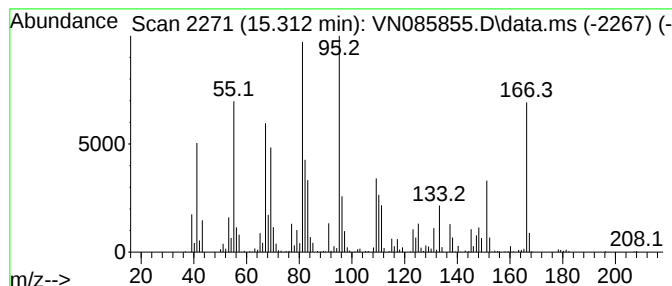
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Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, decahydro-1,2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.312	48.14 ug/l	1201440	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2,6-dimet...	166	C12H22	001618-22-0	98
2			Naphthalene, decahydro-1,2-dimet...	166	C12H22	003604-14-6	90
3			cis,trans-1,6-Dimethylspiro[4.5]...	166	C12H22	1000111-72-3	89
4			trans,trans-1,6-Dimethylspiro[4....	166	C12H22	1000111-72-1	70
5			cis,cis-1,6-Dimethylspiro[4.5]de...	166	C12H22	1000111-72-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

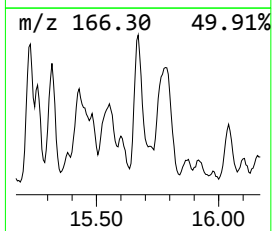
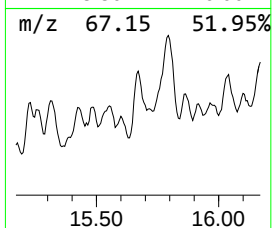
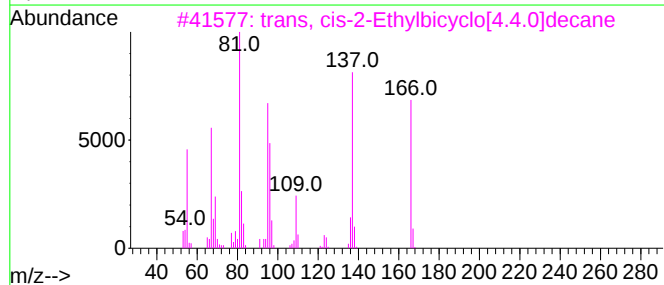
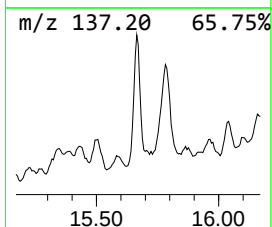
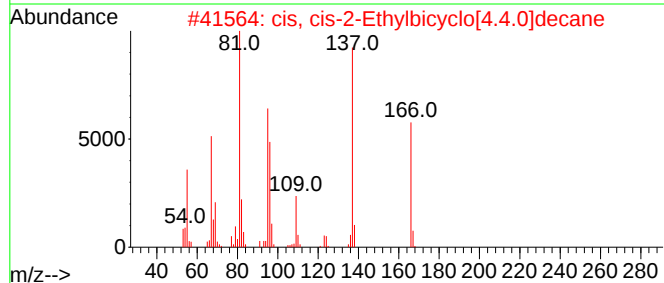
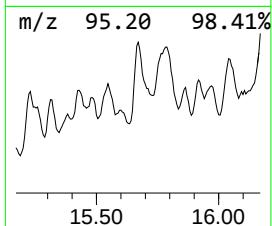
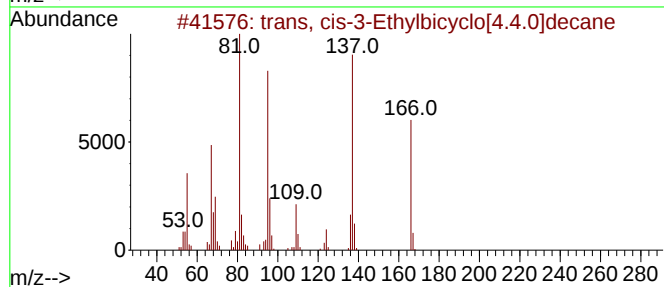
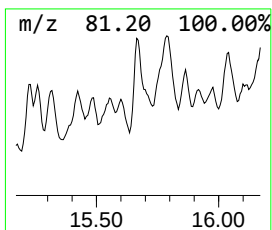
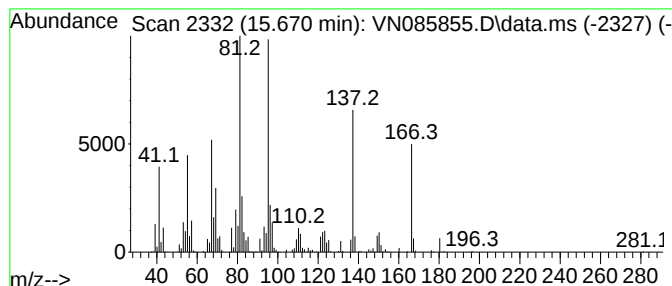
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Quant Title : SW846 8260

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

Peak Number 10 cis, cis-2-Ethylbicyclo[4.4... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.670	118.85 ug/l	2966000	1,4-Dichlorobenzene-d4	13.788

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans, cis-3-Ethylbicyclo[4.4.0]...	166	C12H22	066660-43-3	87
2			cis, cis-2-Ethylbicyclo[4.4.0]de...	166	C12H22	066660-40-0	70
3			trans, cis-2-Ethylbicyclo[4.4.0]...	166	C12H22	066660-39-7	68
4			Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	64
5			Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN022525\
Data File : VN085855.D
Acq On : 25 Feb 2025 14:24
Operator : JC\MD
Sample : Q1395-01
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
BEL-25-0005

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N021825W.M
Quant Title : SW846 8260

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

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					#	RT	Resp	Conc
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Naphthalene, de...	14.118	44.9	ug/l	1120690	4	13.788	1247770	50.0
unknown14.223	14.223	24.0	ug/l	598333	4	13.788	1247770	50.0
Naphthalene, de...	14.623	63.0	ug/l	1572440	4	13.788	1247770	50.0
trans-Decalin, ...	14.794	51.3	ug/l	1278860	4	13.788	1247770	50.0
Bicyclo[3.3.2]d...	14.841	43.6	ug/l	1089170	4	13.788	1247770	50.0
Naphthalene, de...	15.106	72.8	ug/l	1817280	4	13.788	1247770	50.0
trans, cis-3-Et...	15.223	59.9	ug/l	1494510	4	13.788	1247770	50.0
Naphthalene, de...	15.312	48.1	ug/l	1201440	4	13.788	1247770	50.0
cis, cis-2-Ethy...	15.670	118.8	ug/l	2966000	4	13.788	1247770	50.0