

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
 Data File : VN074241.D
 Acq On : 01 Sep 2022 14:41
 Operator : JC\MD
 Sample : N4421-09
 Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 WC-PALM-SP-02-GR

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\82N083022W.M
 Title : SW846 8260

Signal : TIC: VN074241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.404	78	88	98	rBV3	61417	170753	4.65%	0.264%
2	2.751	137	147	148	rBV9	32639	72498	1.97%	0.112%
3	3.322	238	244	252	rVB2	74026	171452	4.67%	0.265%
4	4.769	478	490	504	rBV	71139	236048	6.43%	0.365%
5	5.987	688	697	709	rVB4	44598	136971	3.73%	0.212%
6	7.945	1020	1030	1035	rBV	197070	495702	13.49%	0.765%
7	8.010	1035	1041	1049	rVB	338289	780291	21.24%	1.205%
8	8.210	1067	1075	1082	rBV6	20092	51509	1.40%	0.080%
9	8.363	1093	1101	1113	rBV3	242008	592841	16.14%	0.916%
10	8.492	1115	1123	1127	rBV9	16081	38651	1.05%	0.060%
11	8.745	1161	1166	1172	rVB3	44327	88314	2.40%	0.136%
12	8.898	1183	1192	1203	rBV	530473	1109888	30.21%	1.714%
13	9.386	1265	1275	1281	rBV5	82685	208193	5.67%	0.322%
14	9.663	1315	1322	1326	rBV8	29364	71286	1.94%	0.110%
15	10.333	1430	1436	1438	rBV	157191	274489	7.47%	0.424%
16	10.374	1438	1443	1452	rVB	843614	1583389	43.11%	2.445%
17	10.557	1469	1474	1480	rVB5	59032	123515	3.36%	0.191%
18	10.716	1497	1501	1508	rVB3	78573	144236	3.93%	0.223%
19	10.810	1511	1517	1522	rBV6	49900	111127	3.03%	0.172%
20	10.898	1529	1532	1537	rBV3	35063	55801	1.52%	0.086%
21	10.992	1543	1548	1552	rBV2	77697	141715	3.86%	0.219%
22	11.092	1560	1565	1573	rBV4	72790	178224	4.85%	0.275%
23	11.163	1573	1577	1581	rVV7	45496	86998	2.37%	0.134%
24	11.227	1585	1588	1592	rVV2	83692	120932	3.29%	0.187%
25	11.286	1592	1598	1603	rVB2	202528	357453	9.73%	0.552%
26	11.392	1610	1616	1620	rBV4	112668	218099	5.94%	0.337%
27	11.433	1620	1623	1624	rBV3	47241	48982	1.33%	0.076%
28	11.492	1629	1633	1640	rVV3	139058	278506	7.58%	0.430%
29	11.568	1642	1646	1650	rVB3	90182	161587	4.40%	0.250%
30	11.686	1659	1666	1674	rBV	1019141	1953572	53.18%	3.017%
31	11.780	1679	1682	1684	rBV3	56910	77133	2.10%	0.119%
32	11.821	1686	1689	1692	rVB4	72467	77548	2.11%	0.120%
33	11.892	1692	1701	1704	rBV4	193677	628880	17.12%	0.971%
34	11.927	1704	1707	1711	rVB	171130	253906	6.91%	0.392%
35	12.027	1721	1724	1727	rBV5	62352	98492	2.68%	0.152%
36	12.192	1745	1752	1759	rBV5	549242	1229127	33.46%	1.898%

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37	12.310	1768	1772	1776	rVB	552925	811092	22.08%	1.253%
38	12.392	1776	1786	1788	rBV4	498093	1127710	30.70%	1.741%
39	12.421	1788	1791	1802	rVB3	669705	1444230	39.32%	2.230%
40	12.563	1811	1815	1818	rBV4	213104	292133	7.95%	0.451%
41	12.674	1828	1834	1839	rBV	1394485	2494761	67.92%	3.853%
42	12.833	1857	1861	1869	rVB3	751552	1385248	37.71%	2.139%
43	12.915	1869	1875	1880	rBV5	418704	886719	24.14%	1.369%
44	12.998	1881	1889	1893	rBV4	1083280	2657104	72.34%	4.103%
45	13.133	1909	1912	1916	rVB	539550	723699	19.70%	1.118%
46	13.221	1923	1927	1934	rVB	1278036	1964329	53.48%	3.033%
47	13.351	1946	1949	1953	rBV2	430483	514245	14.00%	0.794%
48	13.404	1954	1958	1961	rBV	473292	657222	17.89%	1.015%
49	13.504	1967	1975	1979	rBV6	1519318	3466051	94.36%	5.352%
50	13.615	1989	1994	2003	rVB3	1386322	3201851	87.16%	4.945%
51	13.757	2014	2018	2023	rBV4	540470	1088151	29.62%	1.680%
52	13.933	2043	2048	2053	rBV2	2111865	3673327	100.00%	5.673%
53	13.980	2053	2056	2060	rVB2	422833	619107	16.85%	0.956%
54	14.257	2099	2103	2109	rVB4	788291	1329400	36.19%	2.053%
55	14.327	2110	2115	2121	rBV6	785282	1451271	39.51%	2.241%
56	14.380	2121	2124	2126	rBV3	324652	471103	12.82%	0.728%
57	14.445	2130	2135	2140	rVV2	2138962	3495201	95.15%	5.398%
58	14.557	2151	2154	2158	rBV6	650232	976864	26.59%	1.509%
59	14.609	2159	2163	2168	rVB4	1241742	1993588	54.27%	3.079%
60	14.792	2191	2194	2199	rVB4	629544	926428	25.22%	1.431%
61	14.857	2201	2205	2210	rVV3	1622377	3246795	88.39%	5.014%
62	14.909	2210	2214	2220	rVB4	1745025	3484837	94.87%	5.382%
63	15.398	2293	2297	2305	rBV3	1296781	2481542	67.56%	3.832%
64	15.809	2364	2367	2374	rVB5	901917	1614514	43.95%	2.493%
65	16.380	2461	2464	2470	rVB5	536670	912320	24.84%	1.409%
66	16.727	2517	2523	2533	rBV6	1052271	2936845	79.95%	4.535%

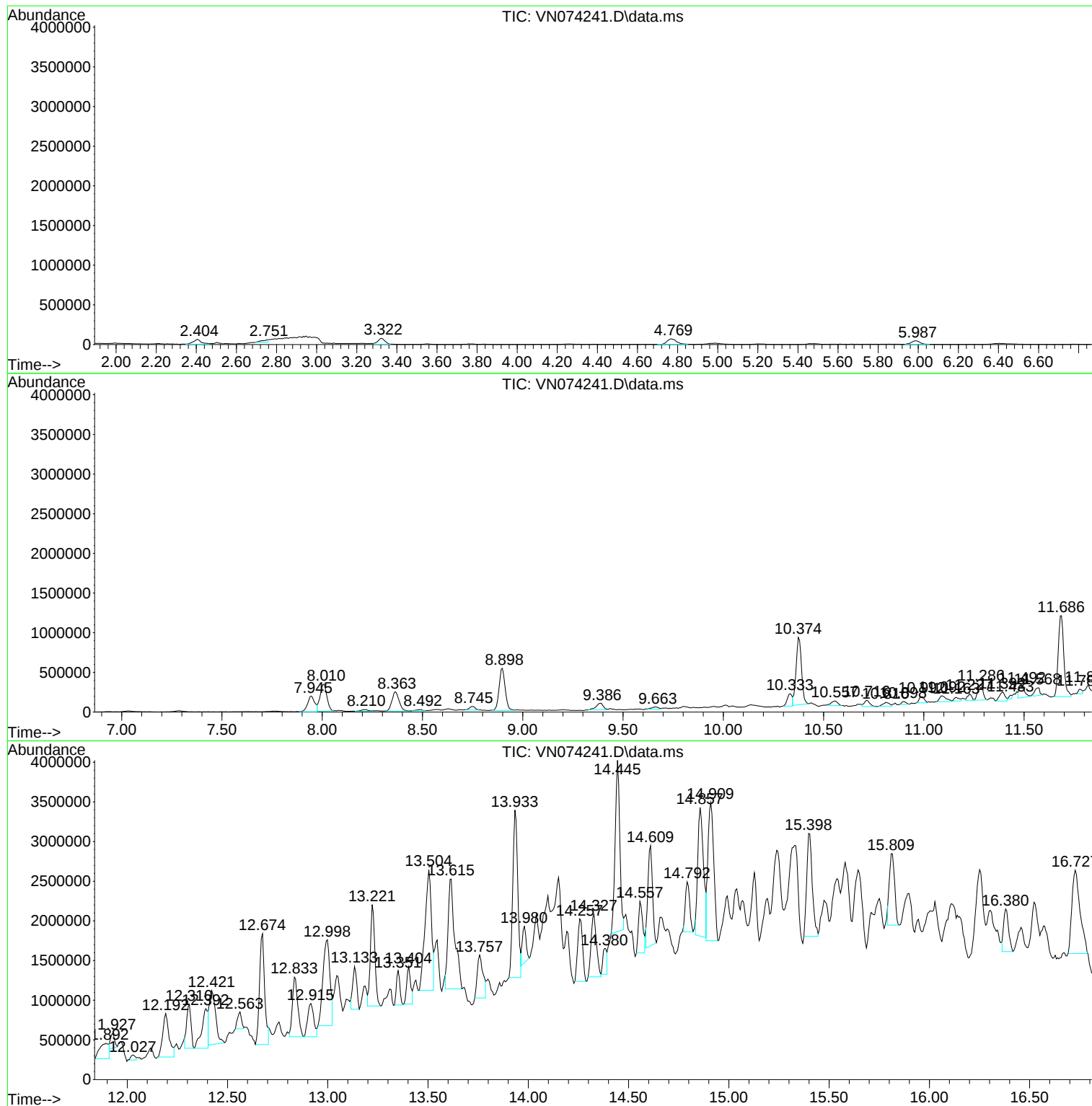
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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



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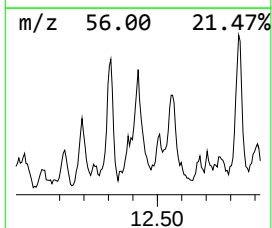
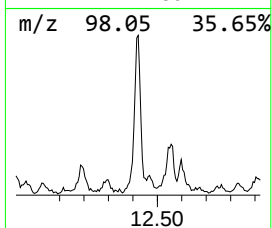
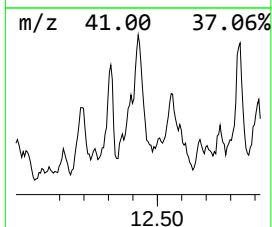
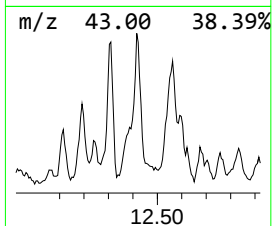
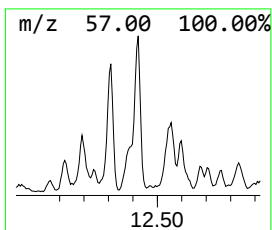
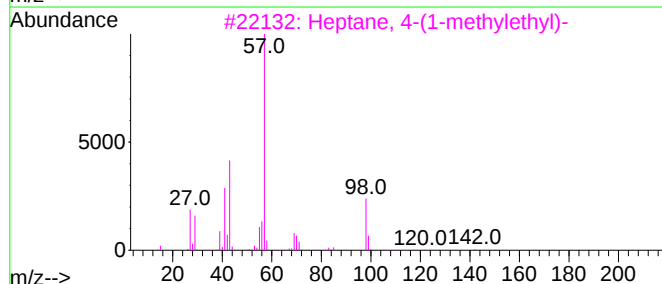
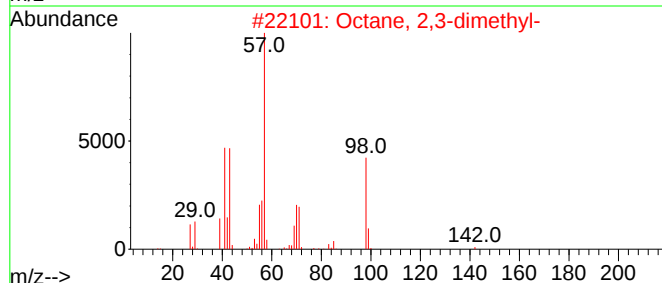
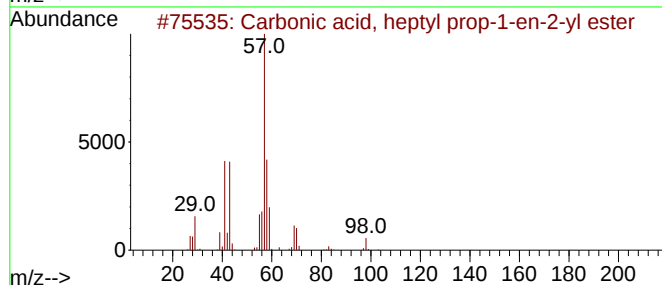
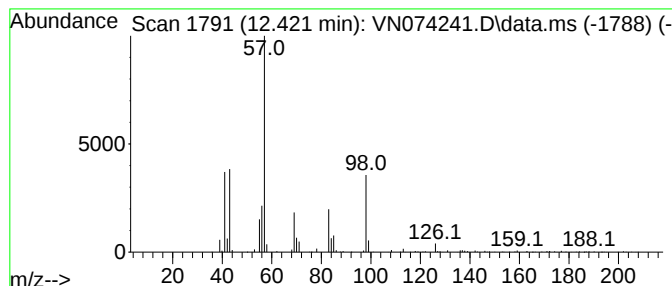
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
Quant Title : SW846 8260

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

Peak Number 1 Carbonic acid, heptyl prop-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	36.96 ug/l	1444230	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	50
2			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47
3			Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	46
4			4-Octylcyclohexanone	210	C14H26O	1000428-94-1	42
5			Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	42



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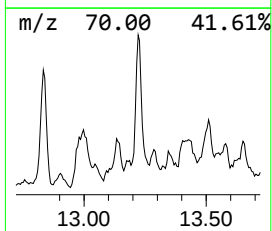
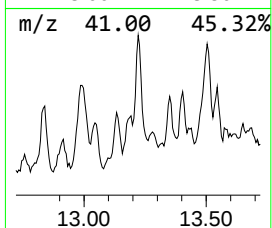
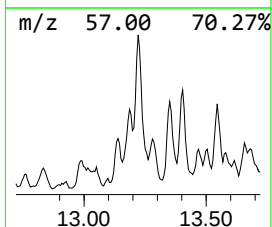
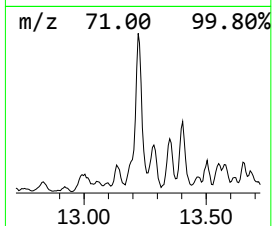
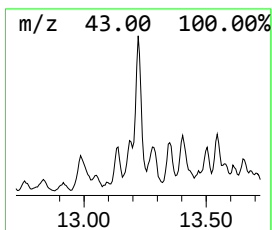
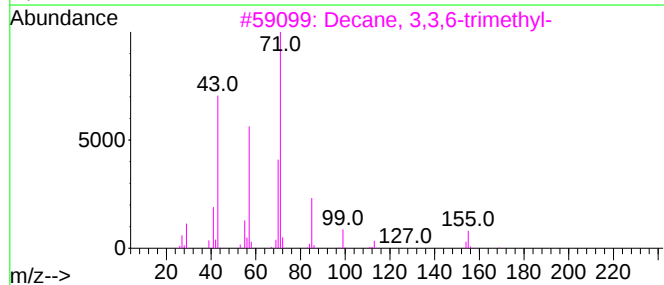
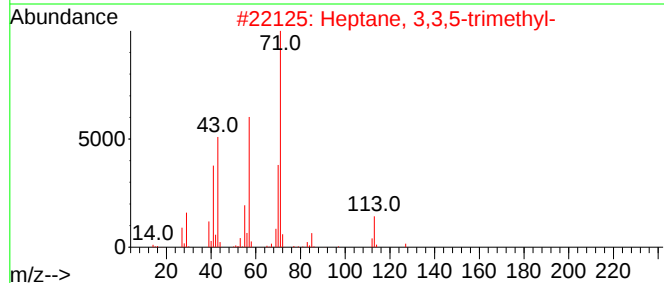
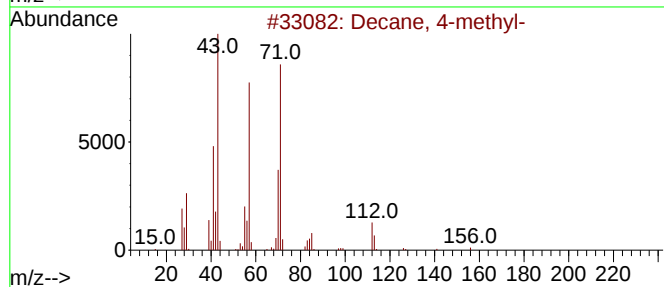
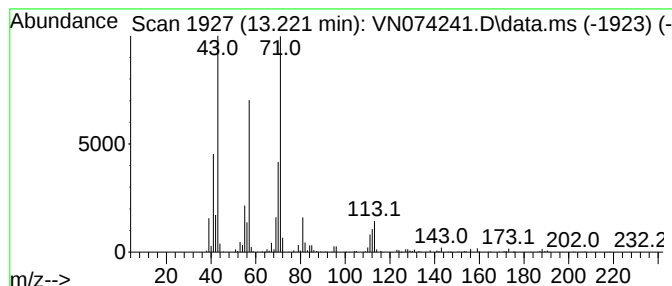
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Decane, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.221	30.67 ug/l	1964330	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	83
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	72
3			Decane, 3,3,6-trimethyl-	184	C13H28	062338-14-1	64
4			2-Propyl-1-pentanol, 2-methylpro...	200	C12H24O2	1000447-36-4	59
5			Dodecane, 4-methyl-	184	C13H28	006117-97-1	59



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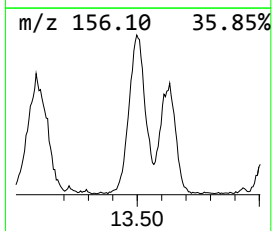
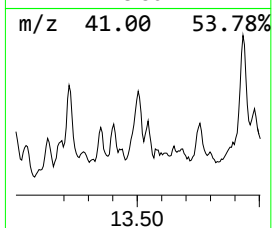
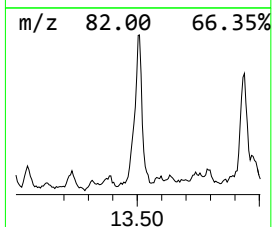
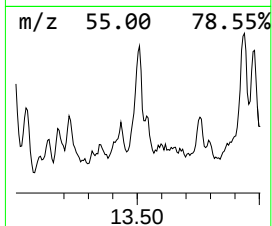
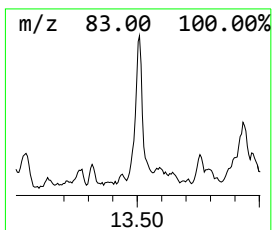
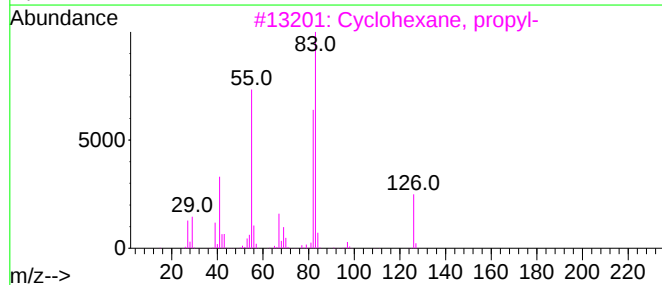
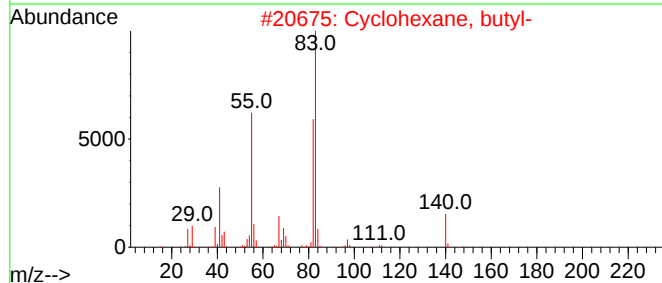
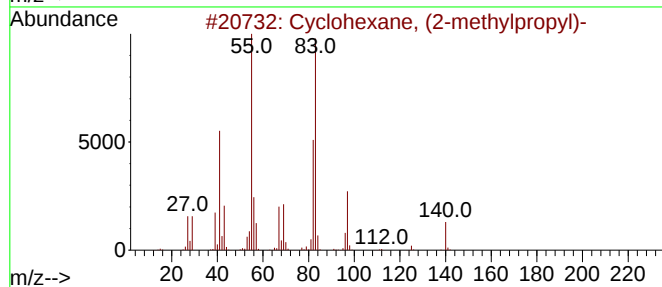
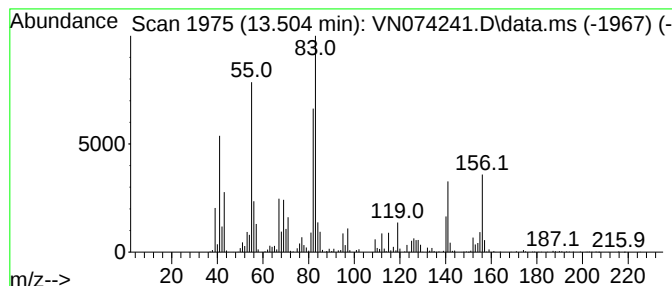
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Peak Number 3 Cyclohexane, (2-methylpropyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.504	54.13 ug/l	3466050	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	58
2			Cyclohexane, butyl-	140	C10H20	001678-93-9	52
3			Cyclohexane, propyl-	126	C9H18	001678-92-8	49
4			Cyclohexane, ethyl-	112	C8H16	001678-91-7	49
5			Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	46



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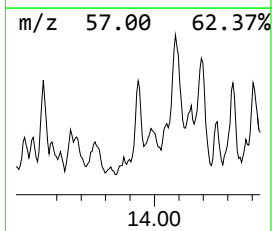
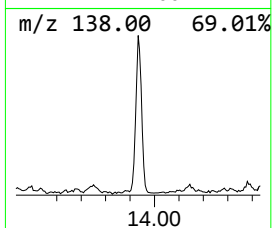
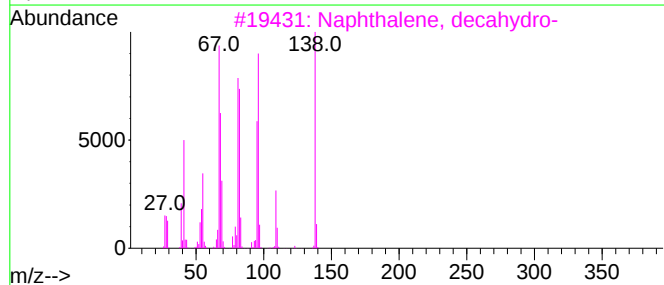
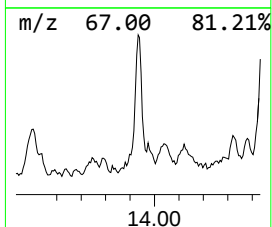
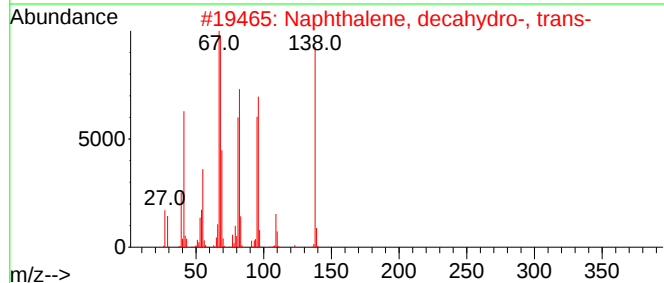
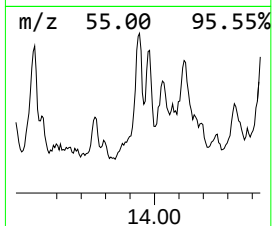
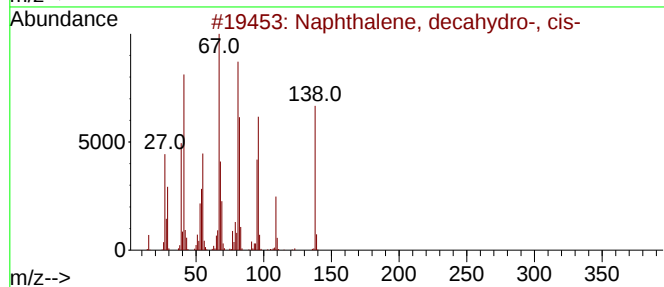
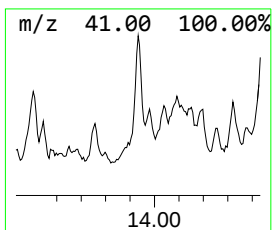
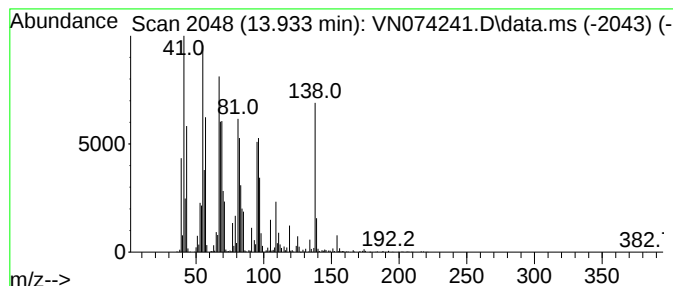
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Peak Number 4 Naphthalene, decahydro-, cis- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.933	57.36 ug/l	3673330	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	95
2			Naphthalene, decahydro-, trans-	138	C10H18	000493-02-7	94
3			Naphthalene, decahydro-	138	C10H18	000091-17-8	89
4			1,1'-Bicyclopentyl	138	C10H18	001636-39-1	76
5			5H-Inden-5-one, octahydro-, cis-	138	C9H14O	004668-91-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

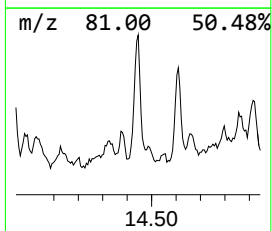
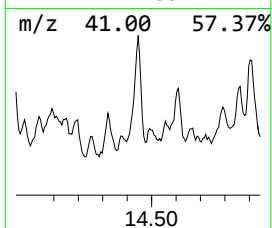
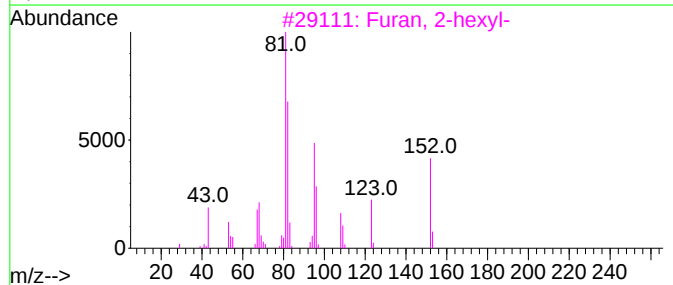
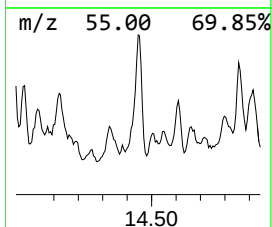
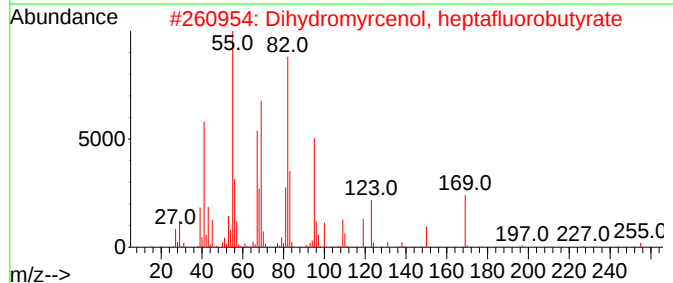
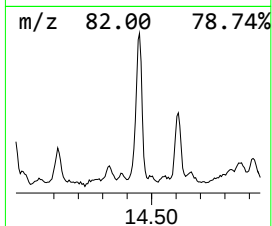
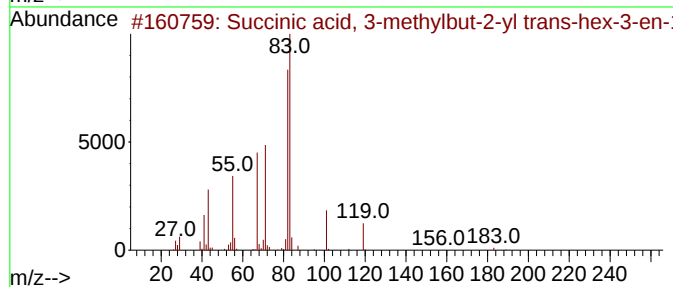
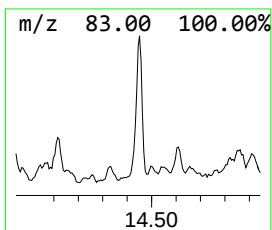
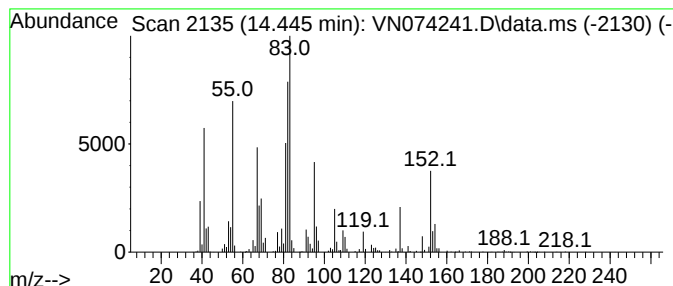
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Quant Title : SW846 8260

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

Peak Number 5 Succinic acid, 3-methylbut-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.445	54.58 ug/l	3495200	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 3-methylbut-2-yl ...	270	C15H26O4	1000391-11-1	50
2			Dihydromyrcenol, heptafluorobuty...	352	C14H19F7O2	1000463-72-0	49
3			Furan, 2-hexyl-	152	C10H16O	003777-70-6	49
4			(Z)-Hex-3-enyl (E)-2-methylbut-2...	182	C11H18O2	067883-79-8	47
5			Cyclohexane, pentyl-	154	C11H22	004292-92-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

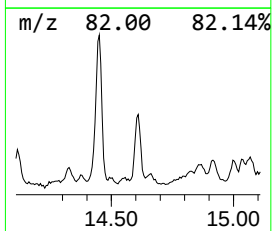
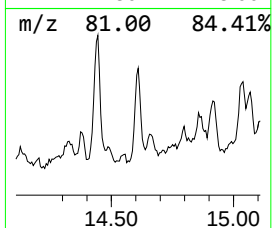
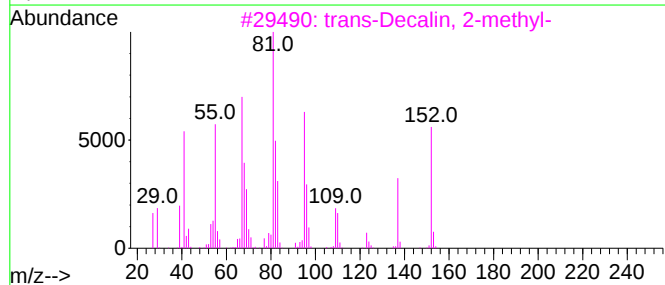
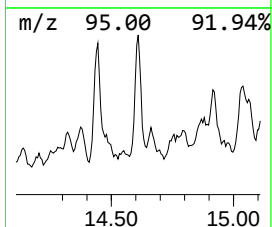
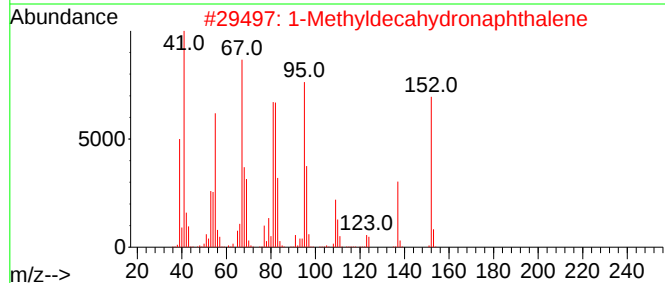
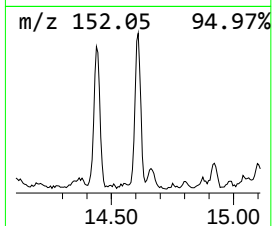
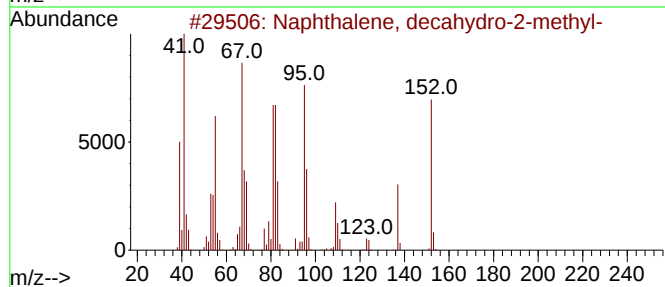
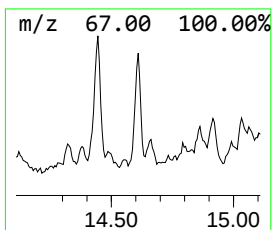
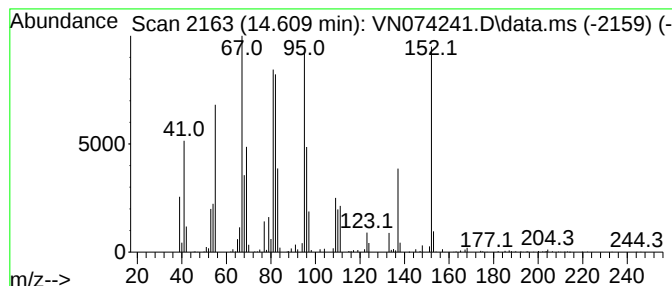
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.610	31.13 ug/l	1993590	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	96
2			1-Methyldecahydronaphthalene	152	C11H20	002958-75-0	96
3			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	70
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	68
5			Decalin, syn-1-methyl-, cis-	152	C11H20	1000158-89-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

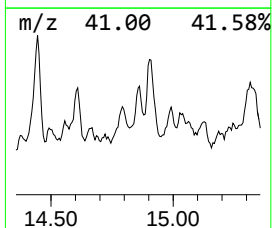
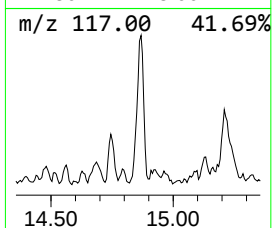
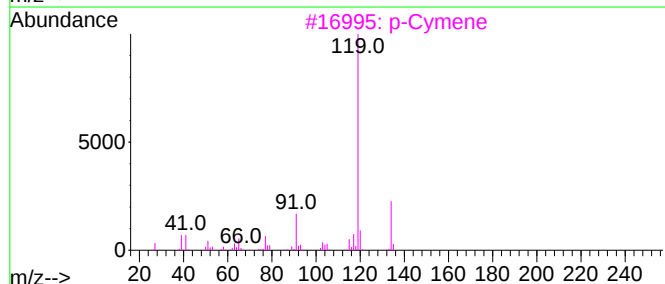
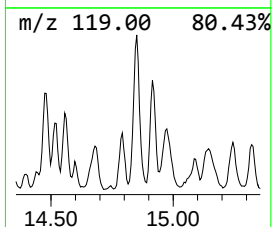
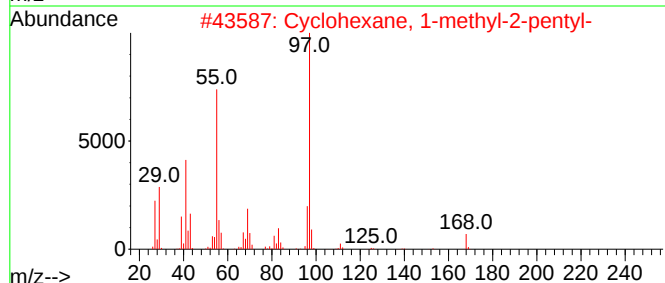
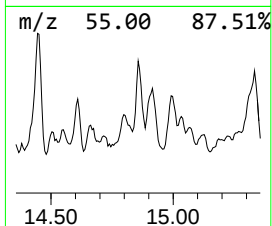
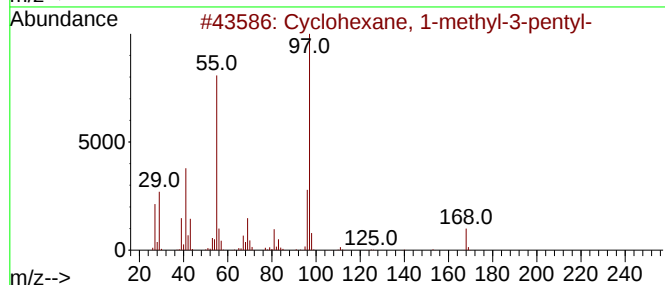
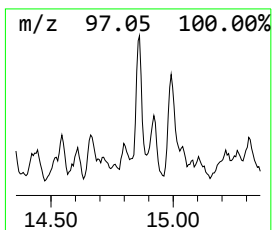
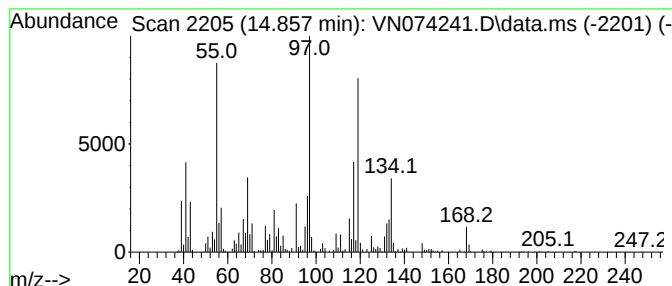
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Quant Title : SW846 8260

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

Peak Number 7 unknown14.857 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	50.70 ug/l	3246800	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-3-pentyl-	168	C12H24	054411-02-8	38
2			Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	38
3			p-Cymene	134	C10H14	000099-87-6	30
4			o-Cymene	134	C10H14	000527-84-4	30
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

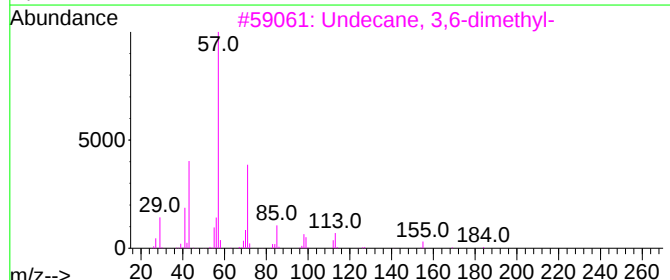
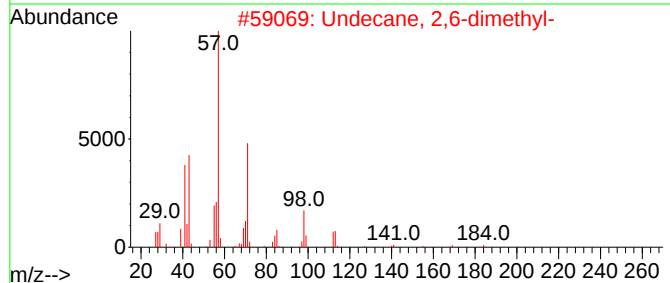
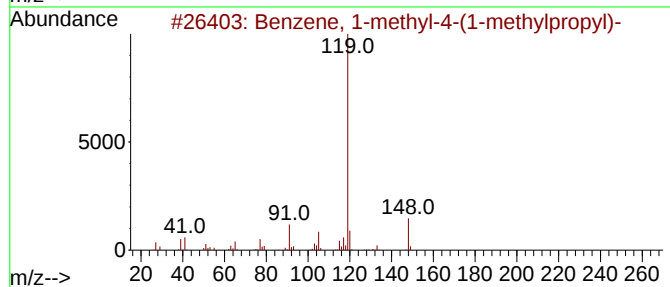
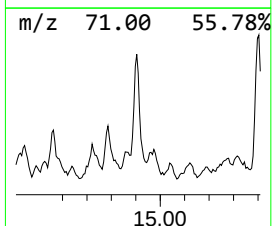
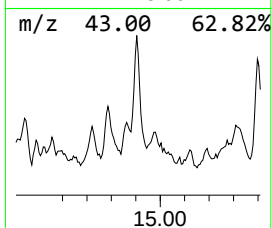
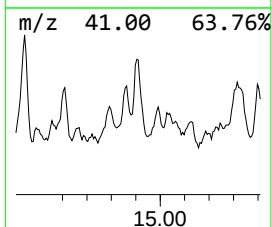
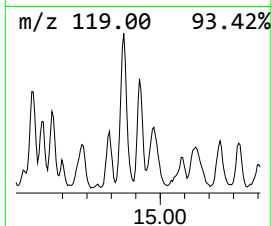
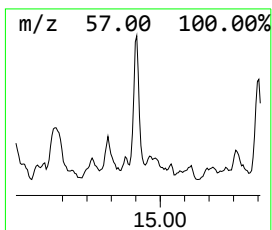
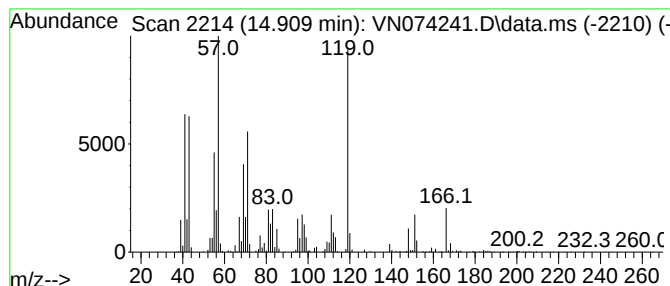
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Quant Title : SW846 8260

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

Peak Number 8 unknown14.910 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.910	54.42 ug/l	3484840	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	30
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	25
3			Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	25
4			Dodecane, 6-methyl-	184	C13H28	006044-71-9	15
5			Octane, 3-ethyl-	142	C10H22	005881-17-4	15



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

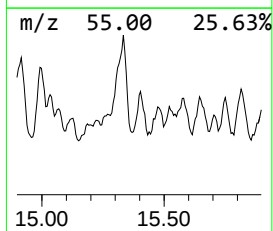
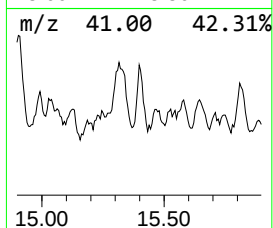
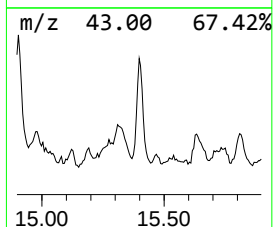
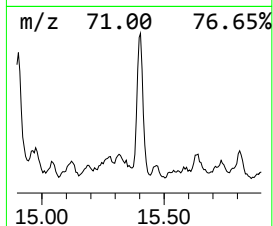
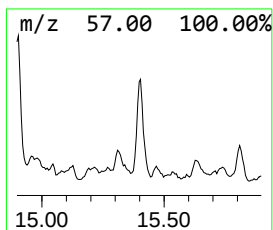
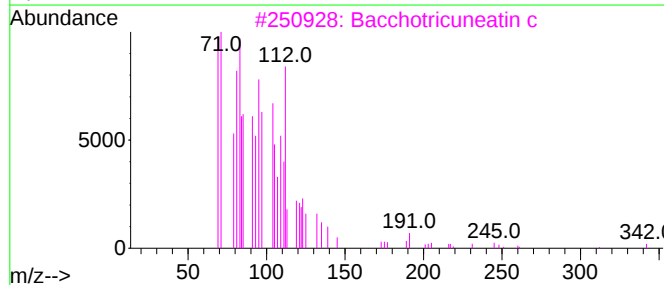
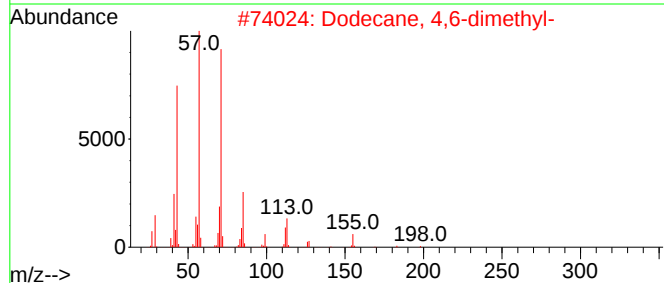
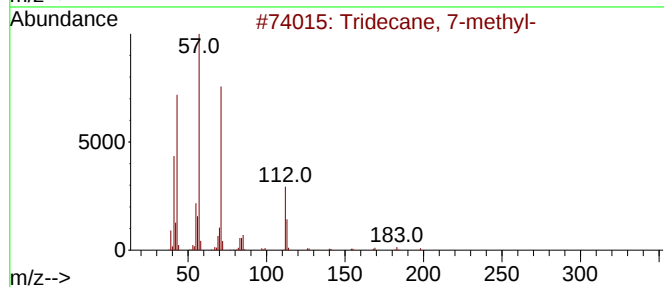
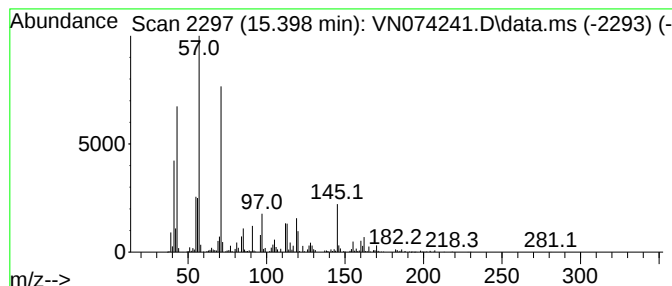
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Quant Title : SW846 8260

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

Peak Number 9 Tridecane, 7-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	38.75 ug/l	2481540	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-methyl-	198	C14H30	026730-14-3	60
2			Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	60
3			Bacchotricuneatin c	342	C20H22O5	066563-30-2	52
4			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	50
5			Octane, 3-ethyl-	142	C10H22	005881-17-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

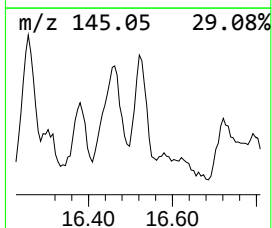
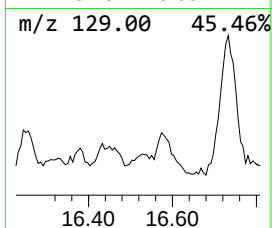
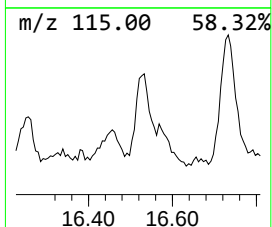
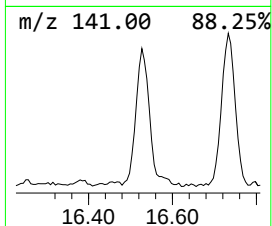
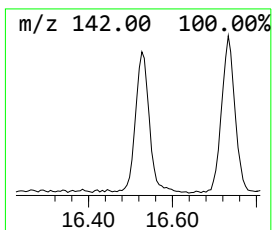
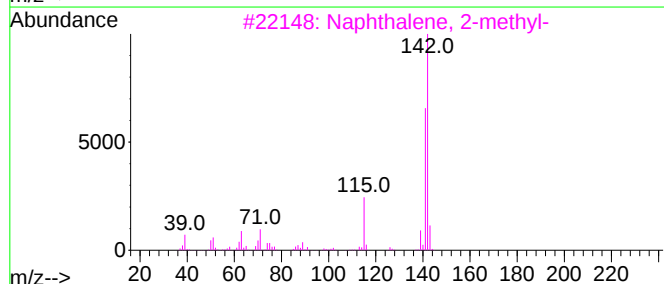
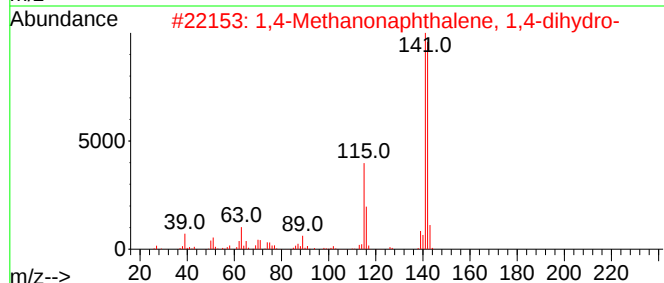
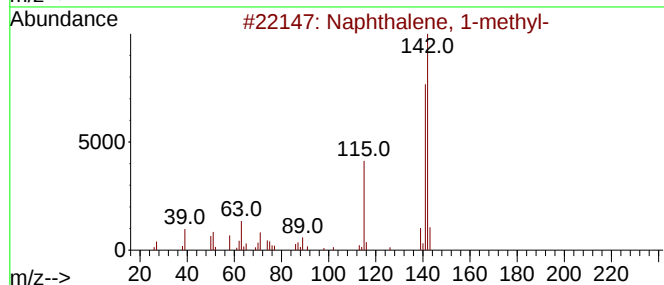
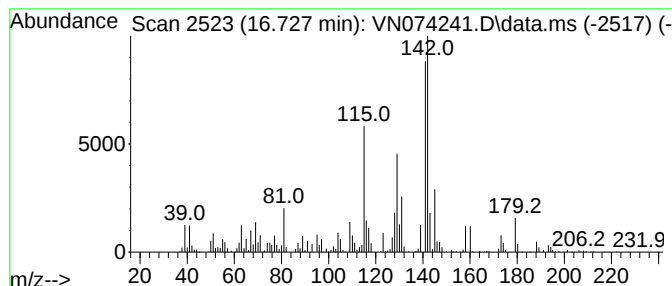
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.727	45.86 ug/l	2936850	1,4-Dichlorobenzene-d4	13.610

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	60
2			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	55
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	53
4			Benzocycloheptatriene	142	C11H10	000264-09-5	47
5			Spiro(tricyclo[6.2.1.0(2,7)]unde...	186	C13H14O	1000210-02-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN090122\
Data File : VN074241.D
Acq On : 01 Sep 2022 14:41
Operator : JC\MD
Sample : N4421-09
Misc : 3.36g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
WC-PALM-SP-02-GR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083022W.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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Decane, 4-methyl-	13.221	30.7	ug/l	1964330	4	13.610	3201850	50.0
Cyclohexane, (2...	13.504	54.1	ug/l	3466050	4	13.610	3201850	50.0
Naphthalene, de...	13.933	57.4	ug/l	3673330	4	13.610	3201850	50.0
Succinic acid, ...	14.445	54.6	ug/l	3495200	4	13.610	3201850	50.0
Naphthalene, de...	14.610	31.1	ug/l	1993590	4	13.610	3201850	50.0
unknown14.857	14.857	50.7	ug/l	3246800	4	13.610	3201850	50.0
unknown14.910	14.910	54.4	ug/l	3484840	4	13.610	3201850	50.0
Tridecane, 7-me...	15.398	38.8	ug/l	2481540	4	13.610	3201850	50.0
Naphthalene, 1-...	16.727	45.9	ug/l	2936850	4	13.610	3201850	50.0