

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
 Data File : VN067275.D
 Acq On : 10 Jun 2021 16:37
 Operator : JC/MD
 Sample : M2644-01
 Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 1846-75-76

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\82N061021W.M
 Title : SW846 8260

Signal : TIC: VN067275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.416	145	159	207	rBV	194897	839519	9.46%	0.683%
2	6.487	1645	1677	1709	rBV3	67046	293503	3.31%	0.239%
3	8.018	2227	2248	2258	rBV2	287551	713880	8.04%	0.580%
4	8.080	2259	2271	2293	rVB2	535371	1255035	14.14%	1.020%
5	8.284	2332	2347	2366	rVB3	59501	140795	1.59%	0.114%
6	8.434	2383	2403	2424	rBV	360243	824652	9.29%	0.670%
7	8.606	2452	2467	2491	rVB2	122743	297903	3.36%	0.242%
8	8.818	2530	2546	2564	rVB3	93736	198108	2.23%	0.161%
9	8.965	2583	2601	2632	rBV	798300	1698026	19.13%	1.381%
10	9.453	2757	2783	2794	rBV3	114924	272068	3.07%	0.221%
11	9.507	2794	2803	2819	rVB3	59182	115809	1.31%	0.094%
12	9.880	2925	2942	2962	rVB2	204108	428810	4.83%	0.349%
13	10.014	2970	2992	3005	rBV2	260158	546357	6.16%	0.444%
14	10.078	3005	3016	3047	rVV3	109171	279576	3.15%	0.227%
15	10.215	3048	3067	3090	rVB3	113517	279064	3.14%	0.227%
16	10.368	3112	3124	3136	rBV2	87671	151227	1.70%	0.123%
17	10.443	3136	3152	3164	rVV	1266252	2446910	27.57%	1.989%
18	10.507	3164	3176	3203	rVV	1326814	2606907	29.38%	2.120%
19	10.623	3205	3219	3234	rVB3	185861	358744	4.04%	0.292%
20	10.883	3304	3316	3336	rVB9	41182	97748	1.10%	0.079%
21	11.054	3361	3380	3391	rBV3	57858	110783	1.25%	0.090%
22	11.154	3407	3417	3435	rBV2	44245	89969	1.01%	0.073%
23	11.347	3479	3489	3502	rVB3	73427	131031	1.48%	0.107%
24	11.457	3518	3530	3539	rBV4	70971	123217	1.39%	0.100%
25	11.527	3540	3556	3582	rVB6	240189	636549	7.17%	0.518%
26	11.628	3582	3594	3607	rBV	226887	376812	4.25%	0.306%
27	11.746	3623	3638	3660	rBV	1097607	2025992	22.83%	1.647%
28	11.848	3663	3676	3694	rBV	420909	766397	8.64%	0.623%
29	11.956	3696	3716	3737	rBV2	2105172	4182272	47.13%	3.400%
30	12.176	3791	3798	3810	rVB8	59435	103750	1.17%	0.084%
31	12.283	3812	3838	3854	rBV2	837130	2069007	23.31%	1.682%
32	12.369	3861	3870	3880	rVB	314139	476852	5.37%	0.388%
33	12.460	3882	3904	3906	rVB6	241068	446080	5.03%	0.363%
34	12.581	3940	3949	3957	rBV3	141835	271765	3.06%	0.221%
35	12.733	3996	4006	4015	rBV	1037528	1709073	19.26%	1.390%
36	12.918	4060	4075	4086	rVB2	377414	831681	9.37%	0.676%

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37	12.983	4086	4099	4107	rBV	1298012	2278309	25.67%	1.852%
38	13.050	4115	4124	4139	rVB3	3141617	5712166	64.37%	4.644%
39	13.112	4141	4147	4158	rVB2	368623	545709	6.15%	0.444%
40	13.224	4172	4189	4203	rBV	565487	1460754	16.46%	1.188%
41	13.286	4205	4212	4227	rVB4	621945	1060867	11.95%	0.863%
42	13.372	4230	4244	4256	rBV	2502922	4172957	47.02%	3.393%
43	13.562	4303	4315	4325	rBV6	988309	1940586	21.87%	1.578%
44	13.608	4327	4332	4340	rVB4	360370	451946	5.09%	0.367%
45	13.675	4349	4357	4364	rBV2	1272143	1887593	21.27%	1.535%
46	13.747	4378	4384	4396	rVB3	422058	547130	6.17%	0.445%
47	13.871	4422	4430	4438	rBV2	1237052	1754414	19.77%	1.426%
48	13.913	4439	4446	4466	rVB4	1388856	2998686	33.79%	2.438%
49	13.997	4466	4477	4489	rBV2	3978588	6280021	70.77%	5.106%
50	14.133	4521	4528	4532	rBV	680003	868795	9.79%	0.706%
51	14.217	4551	4559	4570	rVB	1860152	2838693	31.99%	2.308%
52	14.326	4589	4600	4612	rBV3	1666101	2762706	31.13%	2.246%
53	14.509	4660	4668	4675	rBV6	1492718	2205562	24.85%	1.793%
54	14.581	4689	4695	4703	rVB	1891097	2462746	27.75%	2.002%
55	14.627	4703	4712	4713	rBV2	1569621	1593173	17.95%	1.295%
56	14.654	4715	4722	4740	rVB2	4206487	7874546	88.74%	6.402%
57	14.729	4743	4750	4755	rBV3	566181	798228	8.99%	0.649%
58	14.849	4773	4795	4807	rVB6	3519867	8422616	94.91%	6.848%
59	14.917	4808	4820	4836	rBV5	3192190	8874178	100.00%	7.215%
60	15.088	4877	4884	4899	rVB3	1051283	1867105	21.04%	1.518%
61	15.198	4916	4925	4952	rVB3	1800715	4259982	48.00%	3.464%
62	15.472	5018	5027	5033	rBV5	866030	1498093	16.88%	1.218%
63	15.617	5073	5081	5091	rBV4	1096303	1774193	19.99%	1.442%
64	15.702	5107	5113	5135	rVB4	2058284	3917012	44.14%	3.185%
65	16.021	5224	5232	5246	rVB2	2000444	3646078	41.09%	2.964%
66	16.330	5333	5347	5366	rBV3	2078591	5431687	61.21%	4.416%
67	16.550	5419	5429	5443	rVB4	1287839	2612932	29.44%	2.124%

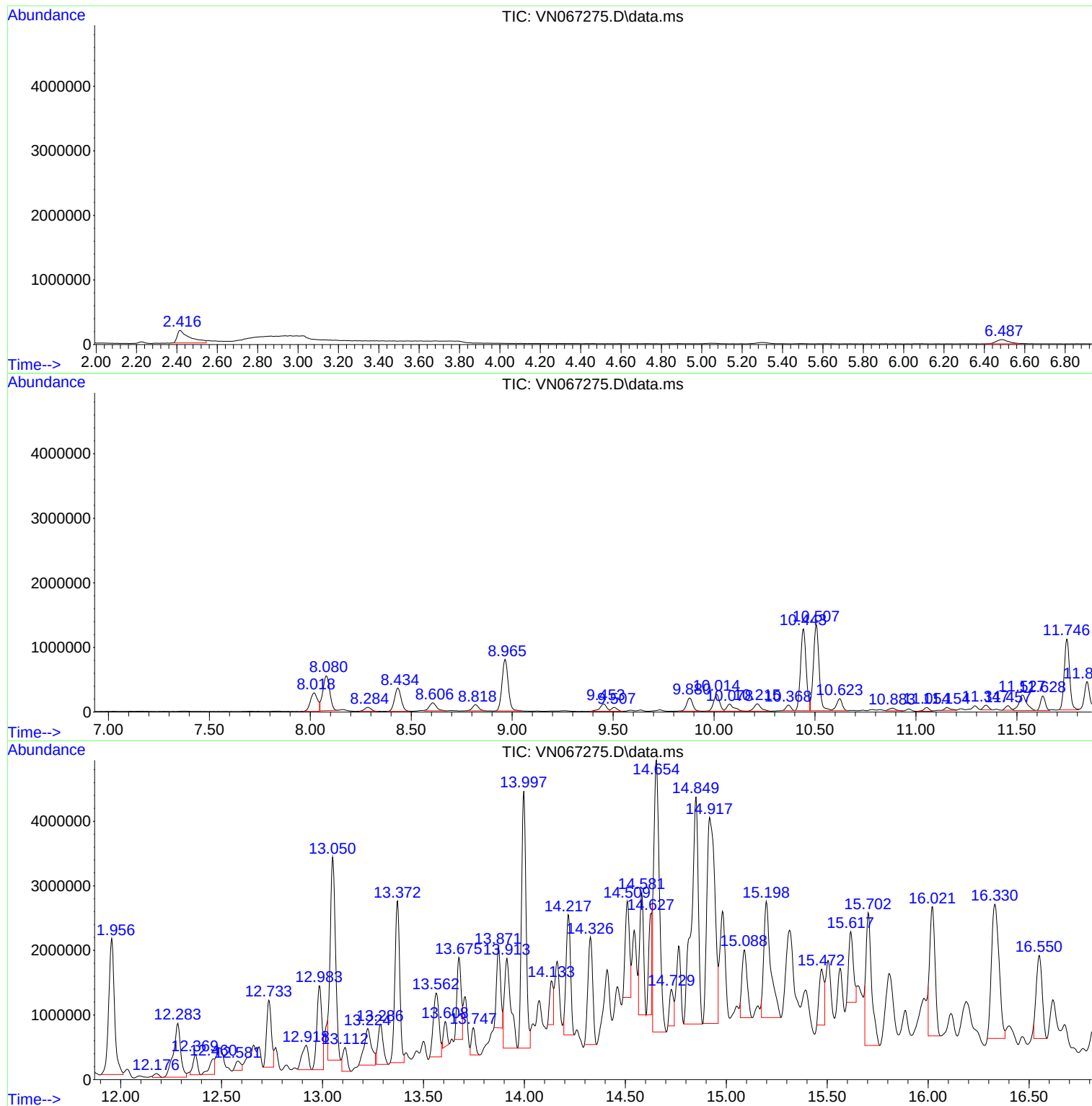
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ClientSampleId :
1846-75-76

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_N
ClientSampleId :
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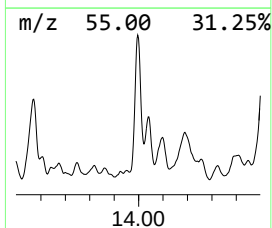
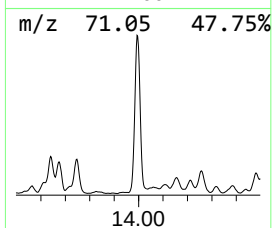
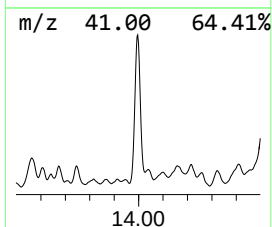
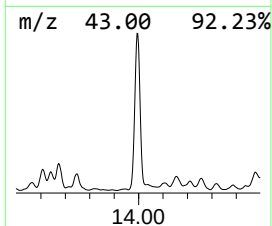
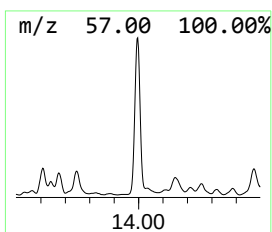
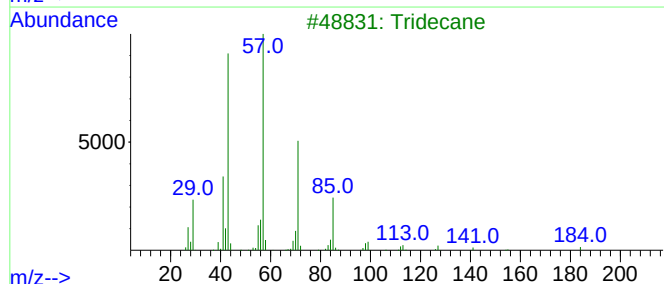
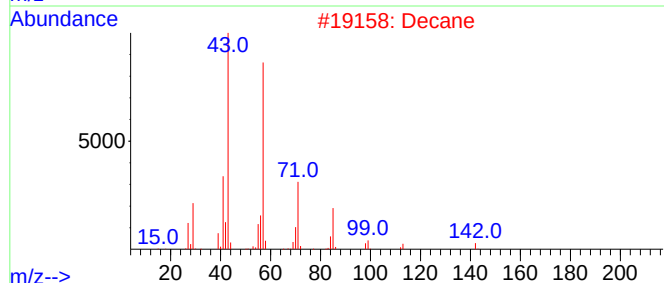
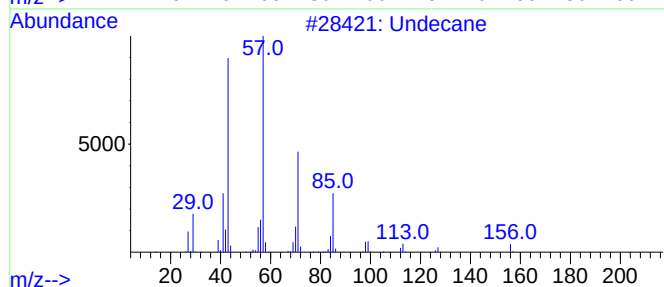
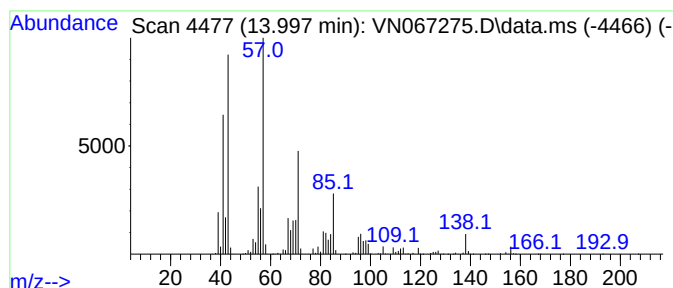
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Undecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.997	166.35 ug/l	6280020	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	81
2	Decane			142	C10H22	000124-18-5	72
3	Tridecane			184	C13H28	000629-50-5	59
4	1-Iodo-2-methylundecane			296	C12H25I	073105-67-6	50
5	Hexadecane			226	C16H34	000544-76-3	50



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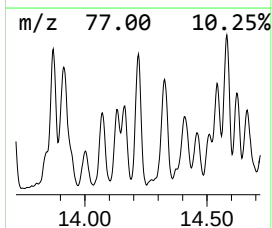
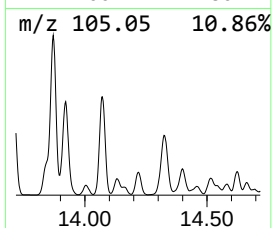
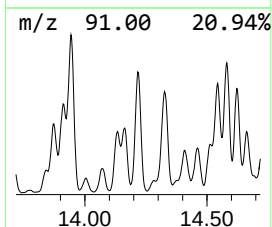
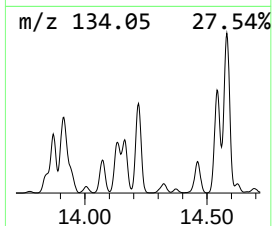
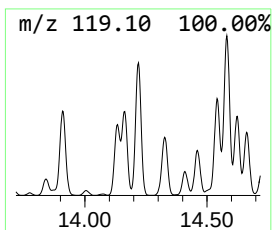
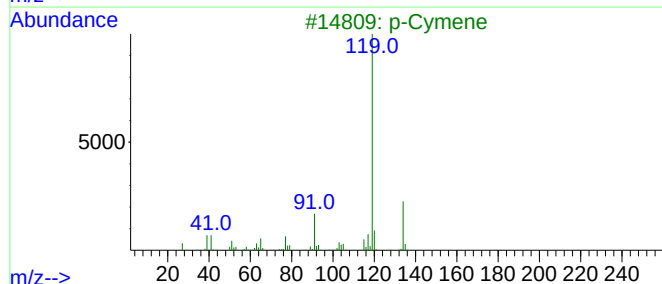
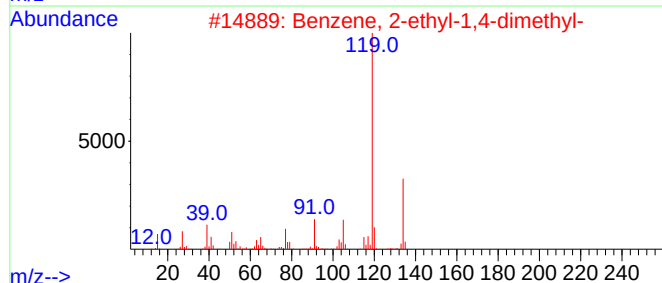
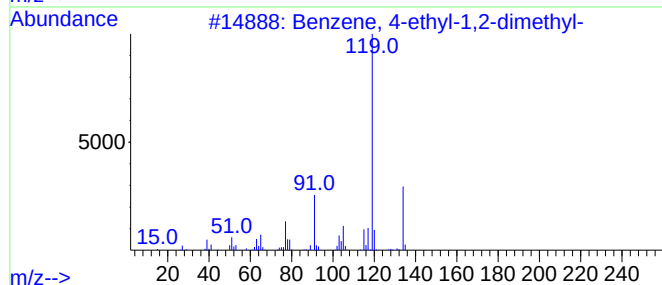
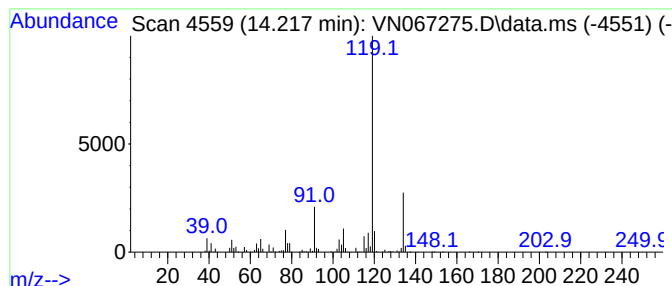
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 4-ethyl-1,2-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	75.19 ug/l	2838690	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	96
2			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
3			p-Cymene	134	C10H14	000099-87-6	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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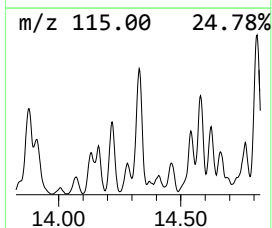
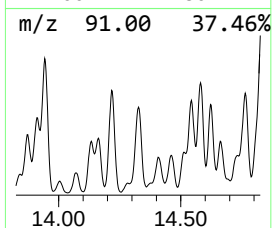
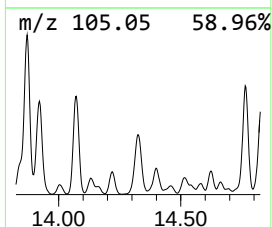
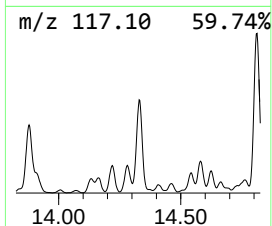
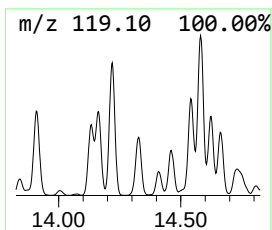
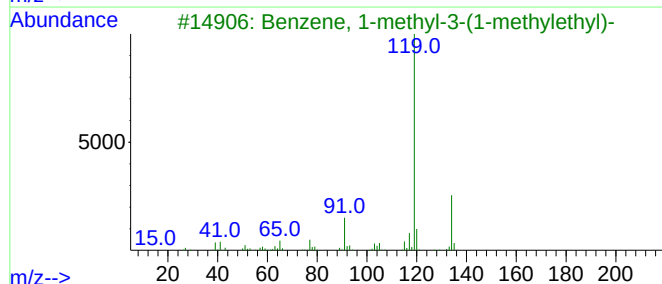
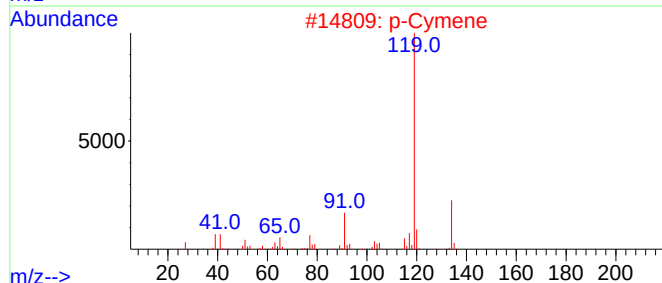
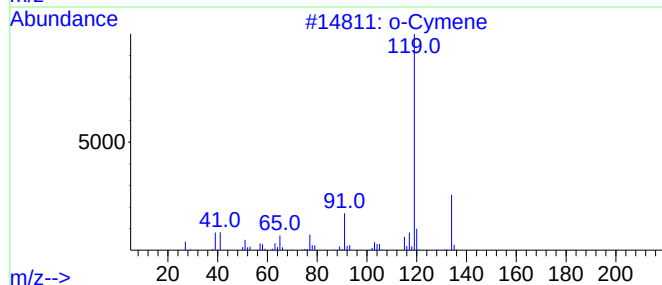
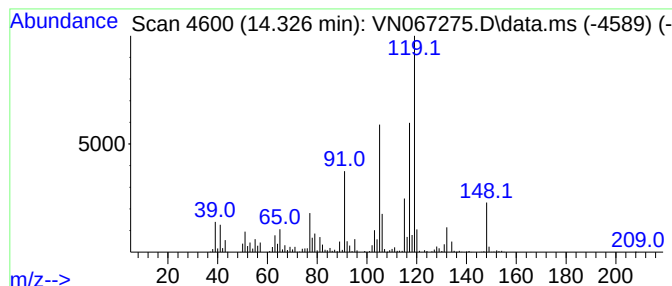
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 o-Cymene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.326	73.18 ug/l	2762710	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Cymene	134	C10H14	000527-84-4	55
2			p-Cymene	134	C10H14	000099-87-6	49
3			Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	000535-77-3	46
4			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	46
5			Propiophenone, 2'-methyl-	148	C10H12O	002040-14-4	43



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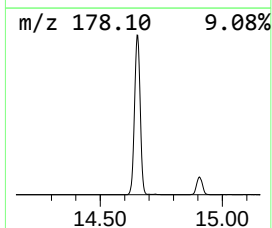
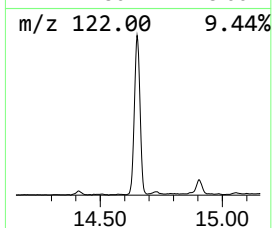
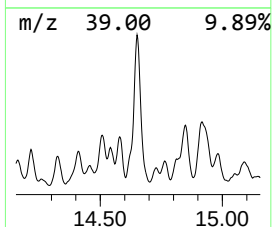
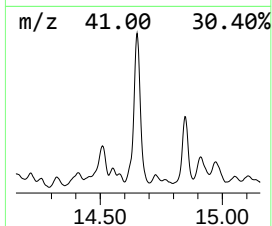
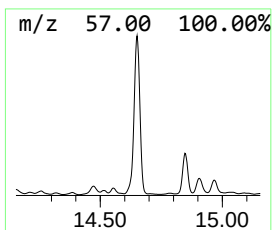
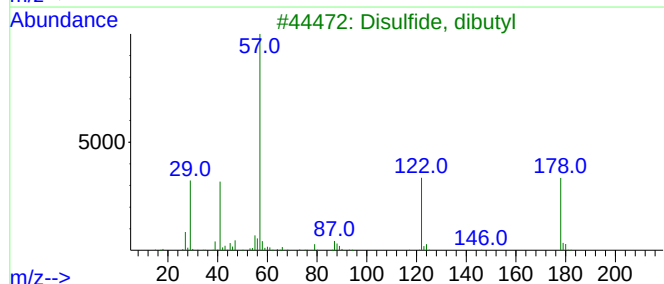
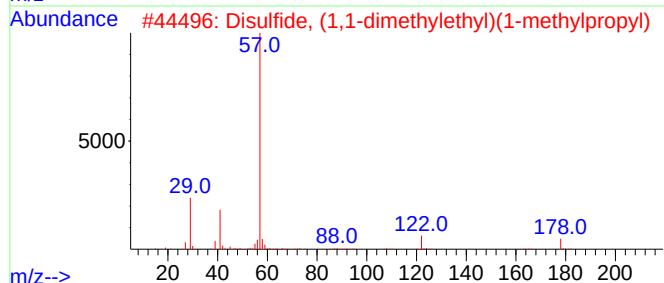
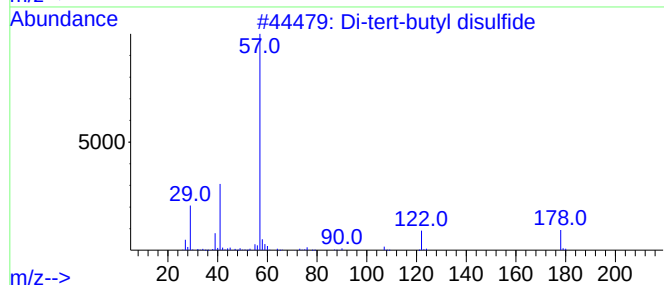
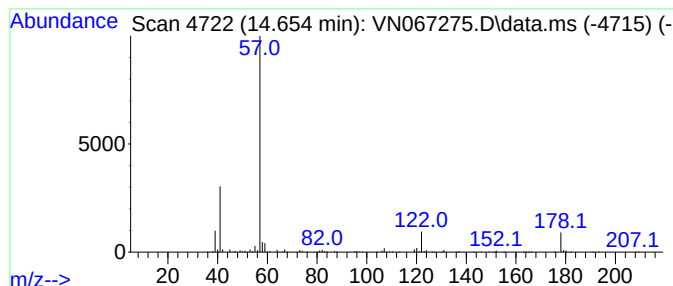
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Di-tert-butyl disulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.654	208.59 ug/l	7874550	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	86
2			Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	80
3			Disulfide, dibutyl	178	C8H18S2	000629-45-8	52
4			Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	35
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

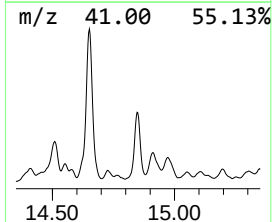
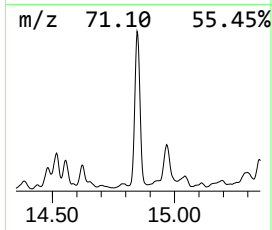
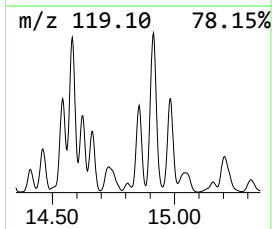
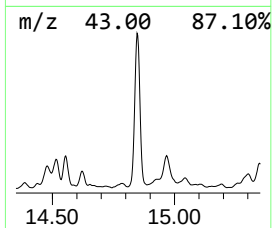
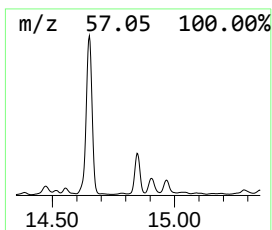
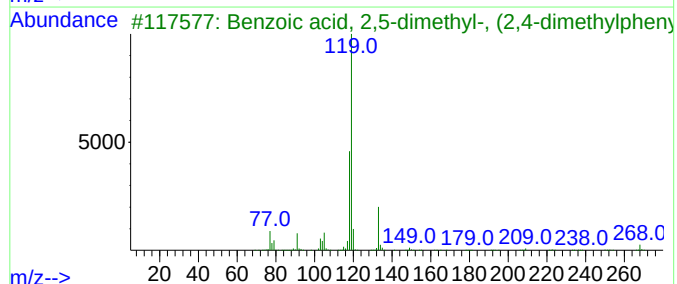
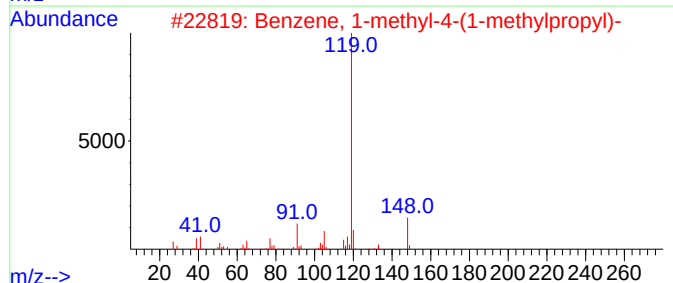
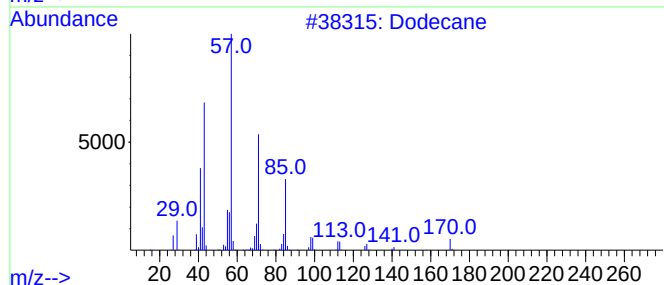
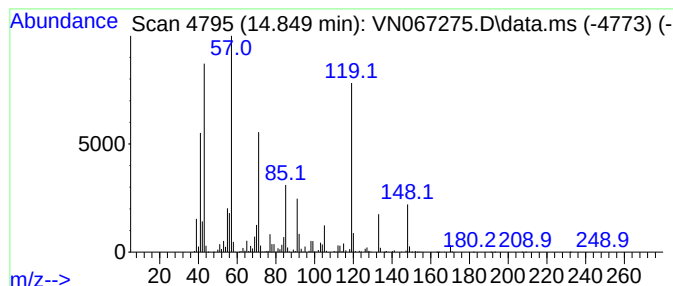
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.850	223.10 ug/l	8422620	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	76
2			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	55
3			Benzoic acid, 2,5-dimethyl-, (2,...	268	C18H20O2	055000-48-1	53
4			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	38
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

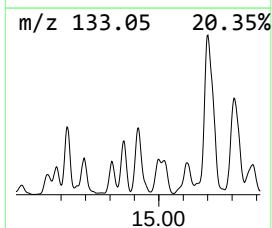
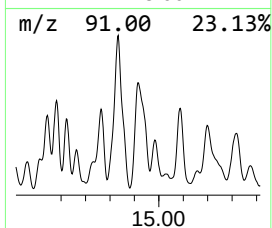
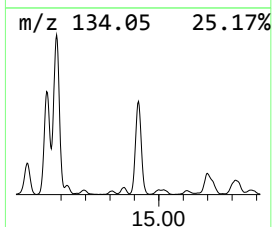
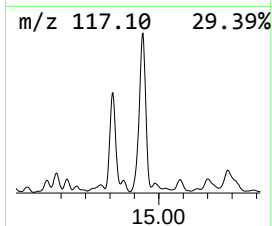
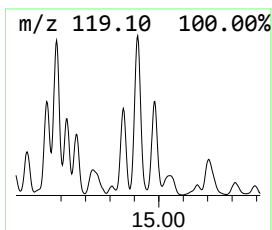
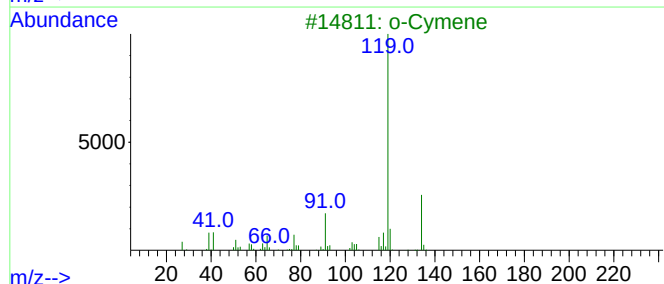
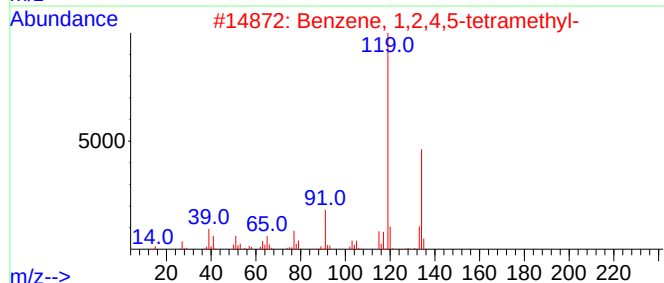
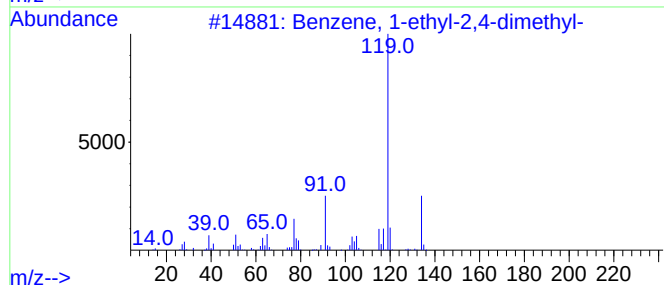
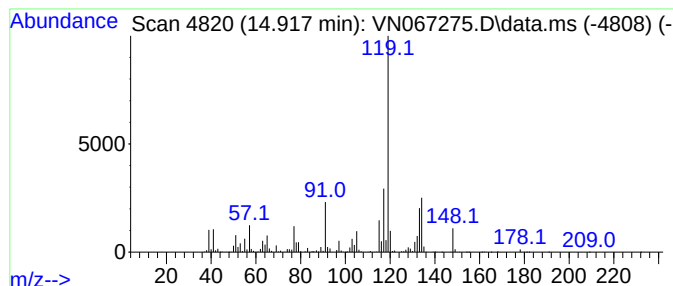
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	235.07 ug/l	8874180	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	92
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	70
3			o-Cymene	134	C10H14	000527-84-4	64
4			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	64
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

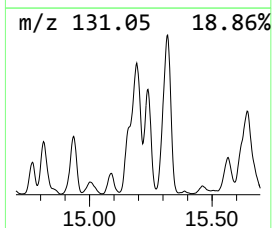
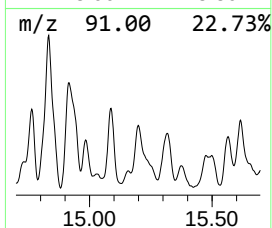
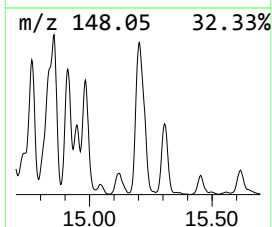
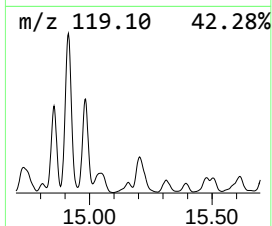
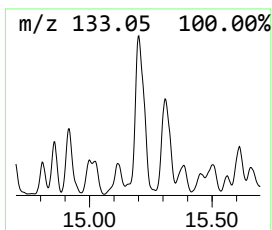
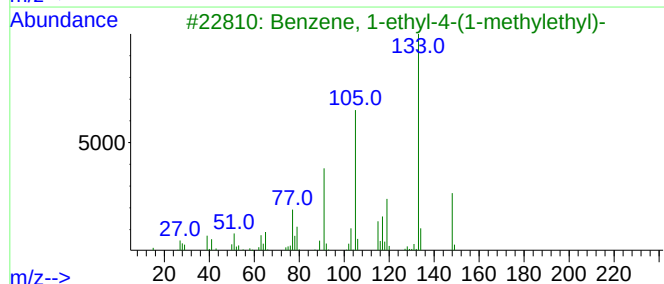
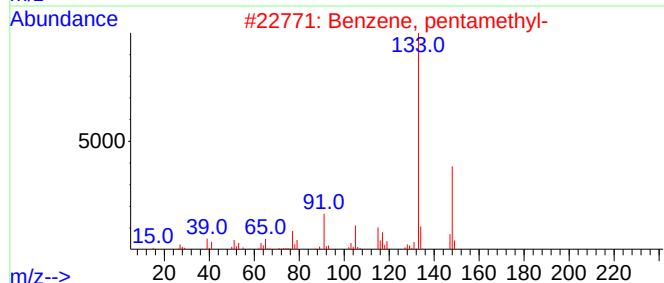
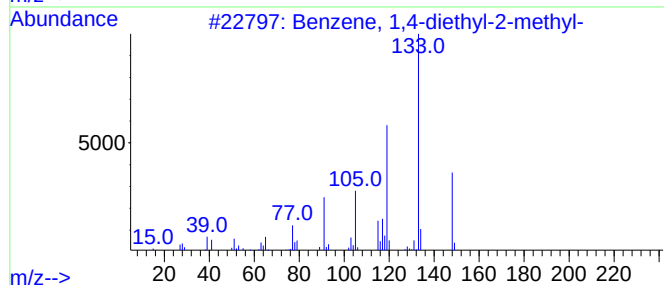
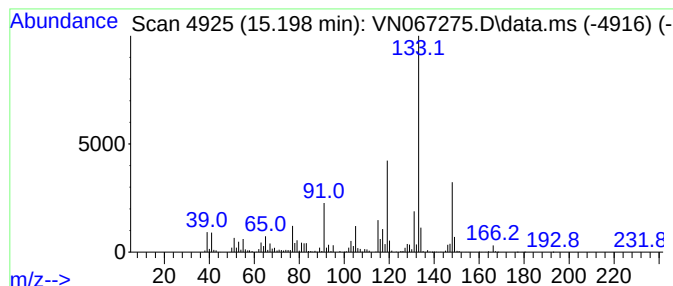
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1,4-diethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	112.84 ug/l	4259980	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,4-diethyl-2-methyl-	148	C11H16	013632-94-5	87
2			Benzene, pentamethyl-	148	C11H16	000700-12-9	70
3			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	64
4			Benzene, 2,4-diethyl-1-methyl-	148	C11H16	001758-85-6	64
5			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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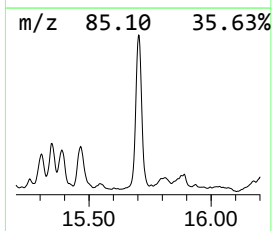
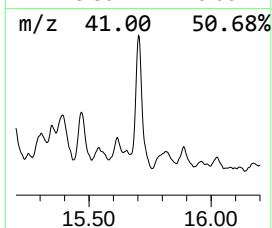
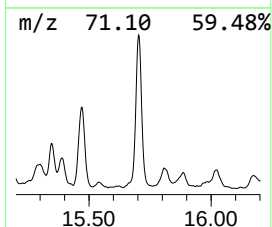
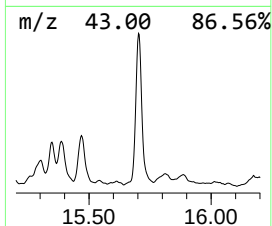
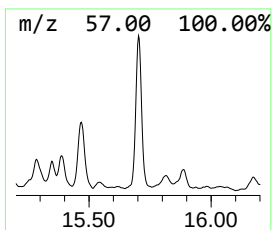
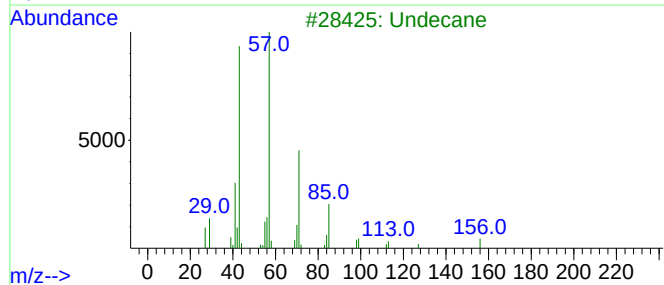
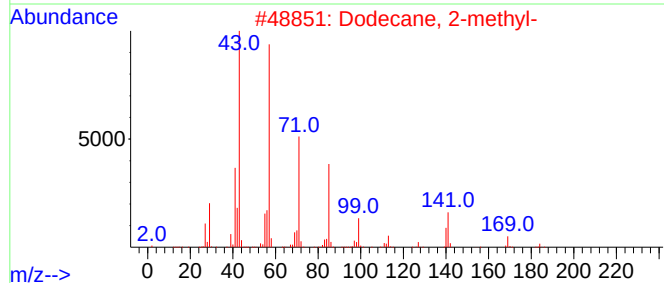
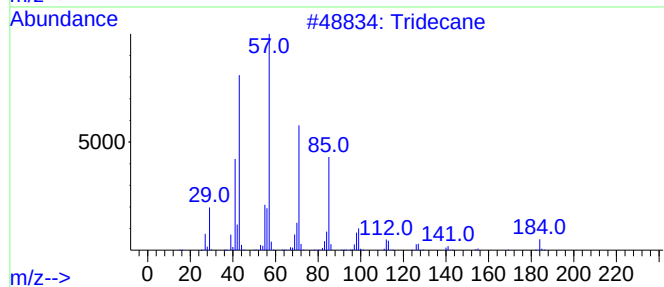
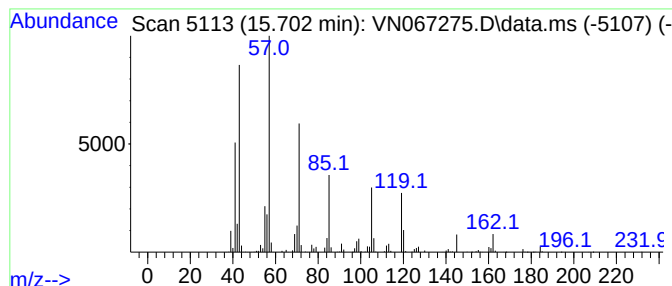
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Tridecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.702	103.76 ug/l	3917010	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	95
2			Dodecane, 2-methyl-	184	C13H28	001560-97-0	49
3			Undecane	156	C11H24	001120-21-4	46
4			Hexadecane	226	C16H34	000544-76-3	46
5			Tetradecane	198	C14H30	000629-59-4	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

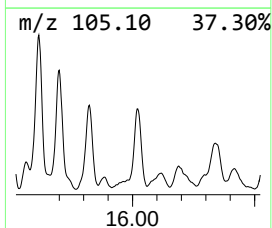
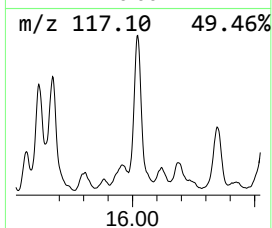
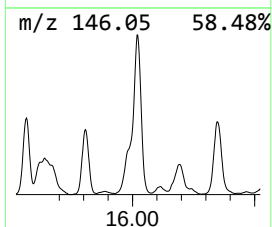
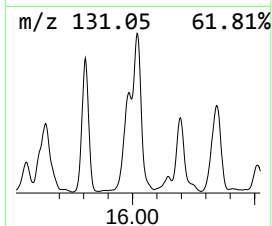
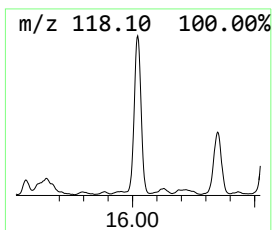
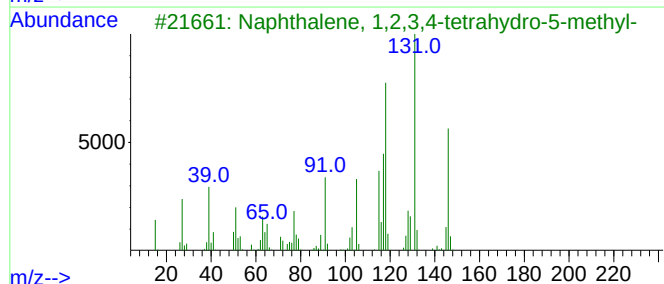
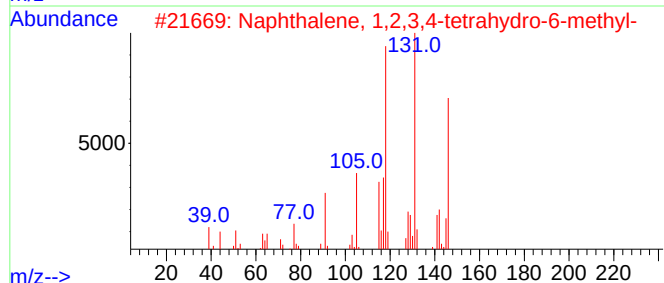
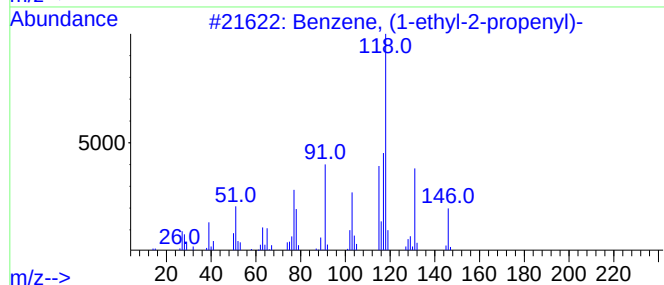
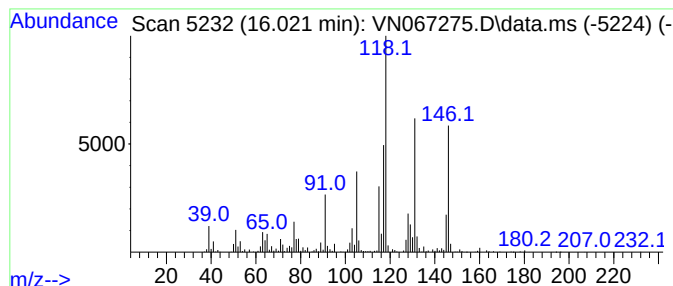
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, (1-ethyl-2-propenyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.022	96.58 ug/l	3646080	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	87
2			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	81
3			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	64
4			Benzene, (1-methylenebutyl)-	146	C11H14	005676-32-4	64
5			Benzene, 2-ethenyl-1,3,5-trimethyl-	146	C11H14	000769-25-5	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

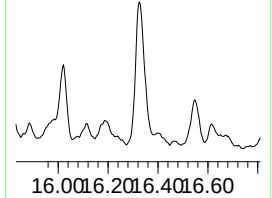
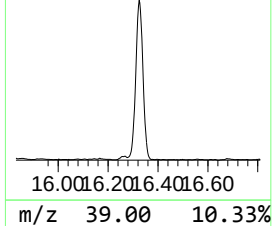
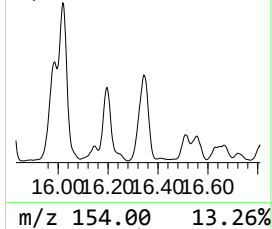
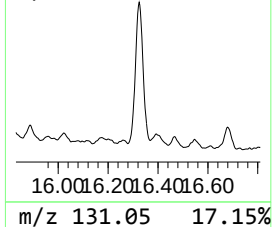
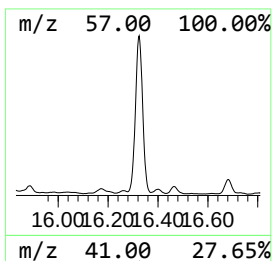
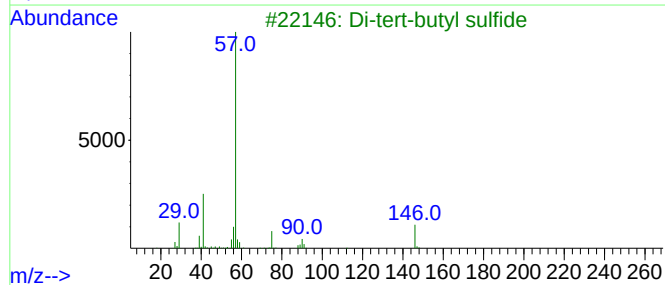
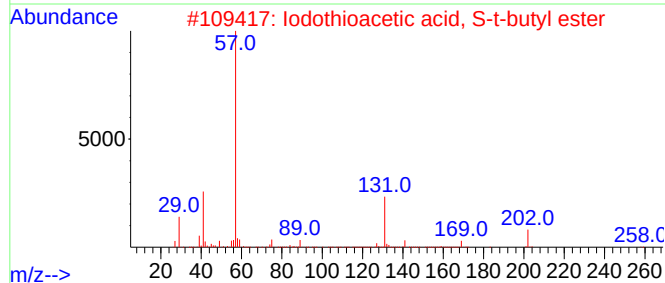
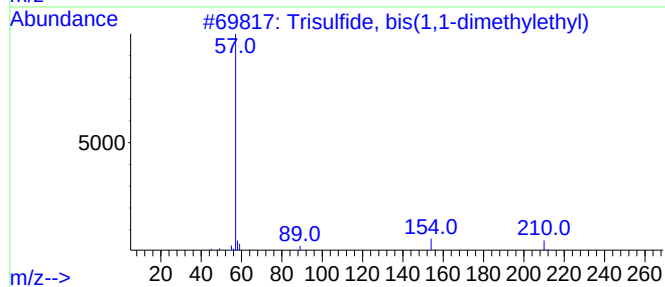
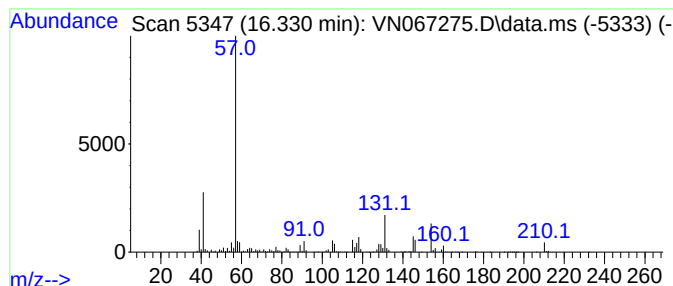
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown16.330 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.330	143.88 ug/l	5431690	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	45
2			Iodothioacetic acid, S-t-butyl e...	258	C6H11IOS	1000192-69-7	27
3			Di-tert-butyl sulfide	146	C8H18S	000107-47-1	12
4			Boc-ON	246	C13H14N2O3	058632-95-4	10
5			Phosphine, bis(1,1-dimethylethyl)-	146	C8H19P	000819-19-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN061021\
Data File : VN067275.D
Acq On : 10 Jun 2021 16:37
Operator : JC/MD
Sample : M2644-01
Misc : 1.15g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1846-75-76

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061021W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 4-ethy...	14.217	75.2	ug/l	2838690	4	13.678	1887590	50.0
o-Cymene	14.326	73.2	ug/l	2762710	4	13.678	1887590	50.0
Di-tert-butyl d...	14.654	208.6	ug/l	7874550	4	13.678	1887590	50.0
Dodecane	14.850	223.1	ug/l	8422620	4	13.678	1887590	50.0
Benzene, 1-ethy...	14.916	235.1	ug/l	8874180	4	13.678	1887590	50.0
Benzene, 1,4-di...	15.198	112.8	ug/l	4259980	4	13.678	1887590	50.0
Tridecane	15.702	103.8	ug/l	3917010	4	13.678	1887590	50.0
Benzene, (1-eth...	16.022	96.6	ug/l	3646080	4	13.678	1887590	50.0
unknown16.330	16.330	143.9	ug/l	5431690	4	13.678	1887590	50.0