

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
 Data File : VN069781.D
 Acq On : 6 Dec 2021 14:10
 Operator : JC/MD
 Sample : M4866-01 10X
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41679

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\82N120221W.M
 Title : SW846 8260

Signal : TIC: VN069781.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	81	92	105	rBV4	56572	117734	1.38%	0.166%
2	2.783	271	296	298	rBV5	60507	162874	1.91%	0.230%
3	8.021	2223	2249	2260	rBV2	948772	2309517	27.12%	3.256%
4	8.086	2261	2273	2299	rVB	1765206	4057998	47.65%	5.722%
5	8.437	2382	2404	2429	rBV	1160339	2697060	31.67%	3.803%
6	8.968	2581	2602	2649	rBV	2835504	5875884	69.00%	8.285%
7	9.459	2760	2785	2797	rBV5	53812	132132	1.55%	0.186%
8	10.443	3133	3152	3167	rBV	4581209	8515557	100.00%	12.007%
9	10.505	3168	3175	3189	rVB2	191155	346463	4.07%	0.489%
10	10.623	3206	3219	3235	rVB3	102690	208351	2.45%	0.294%
11	10.877	3299	3314	3332	rBV8	38284	87142	1.02%	0.123%
12	11.293	3452	3469	3479	rVV2	47875	91519	1.07%	0.129%
13	11.344	3480	3488	3502	rVB4	50219	91716	1.08%	0.129%
14	11.529	3540	3557	3582	rVB7	117213	315844	3.71%	0.445%
15	11.628	3582	3594	3605	rBV2	110000	177976	2.09%	0.251%
16	11.746	3620	3638	3662	rBV	4673976	8412730	98.79%	11.862%
17	11.846	3664	3675	3686	rVV	160675	262649	3.08%	0.370%
18	11.953	3696	3715	3737	rBV3	972885	1996337	23.44%	2.815%
19	12.280	3812	3837	3854	rBV3	394649	986286	11.58%	1.391%
20	12.369	3862	3870	3881	rVB3	100301	147913	1.74%	0.209%
21	12.454	3893	3902	3906	rBV6	65644	95574	1.12%	0.135%
22	12.578	3940	3948	3956	rBV4	66758	114602	1.35%	0.162%
23	12.733	3993	4006	4029	rVB	3682421	6577482	77.24%	9.274%
24	12.918	4061	4075	4086	rVB	195003	386800	4.54%	0.545%
25	12.983	4086	4099	4107	rBV	648934	1120690	13.16%	1.580%
26	13.050	4115	4124	4139	rVB2	1314223	2348405	27.58%	3.311%
27	13.222	4173	4188	4202	rBV	270966	619927	7.28%	0.874%
28	13.286	4204	4212	4228	rVB6	233350	395467	4.64%	0.558%
29	13.369	4230	4243	4255	rBV	1259059	2053643	24.12%	2.896%
30	13.562	4305	4315	4324	rBV7	243333	391872	4.60%	0.553%
31	13.608	4325	4332	4339	rBV4	158271	208982	2.45%	0.295%
32	13.675	4345	4357	4377	rVB2	3964696	7195065	84.49%	10.145%
33	13.871	4422	4430	4438	rBV2	408400	622812	7.31%	0.878%
34	13.994	4466	4476	4488	rBV3	1295522	2001812	23.51%	2.823%
35	14.133	4521	4528	4532	rBV	198749	255711	3.00%	0.361%
36	14.217	4550	4559	4569	rVB2	451756	664889	7.81%	0.938%

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37	14.327	4589	4600	4612	rVB2	434295	708322	8.32%	0.999%
38	14.509	4662	4668	4676	rVB7	238296	275714	3.24%	0.389%
39	14.579	4689	4694	4702	rVB2	360120	447201	5.25%	0.631%
40	14.622	4703	4710	4718	rVV3	312435	397045	4.66%	0.560%
41	14.667	4719	4727	4740	rVB4	257232	439991	5.17%	0.620%
42	14.812	4772	4781	4785	rBV2	354307	503777	5.92%	0.710%
43	14.847	4788	4794	4808	rVB4	889524	1363923	16.02%	1.923%
44	14.927	4810	4824	4836	rBV5	766929	1869142	21.95%	2.636%
45	15.088	4877	4884	4897	rVB	298835	506867	5.95%	0.715%
46	15.195	4916	4924	4934	rBV5	293740	437901	5.14%	0.617%
47	15.469	5019	5026	5031	rBV7	160636	230376	2.71%	0.325%
48	15.617	5074	5081	5090	rBV7	193947	287419	3.38%	0.405%
49	15.702	5107	5113	5134	rVB3	553415	1031401	12.11%	1.454%
50	16.617	5446	5454	5468	rVB4	210912	374779	4.40%	0.528%

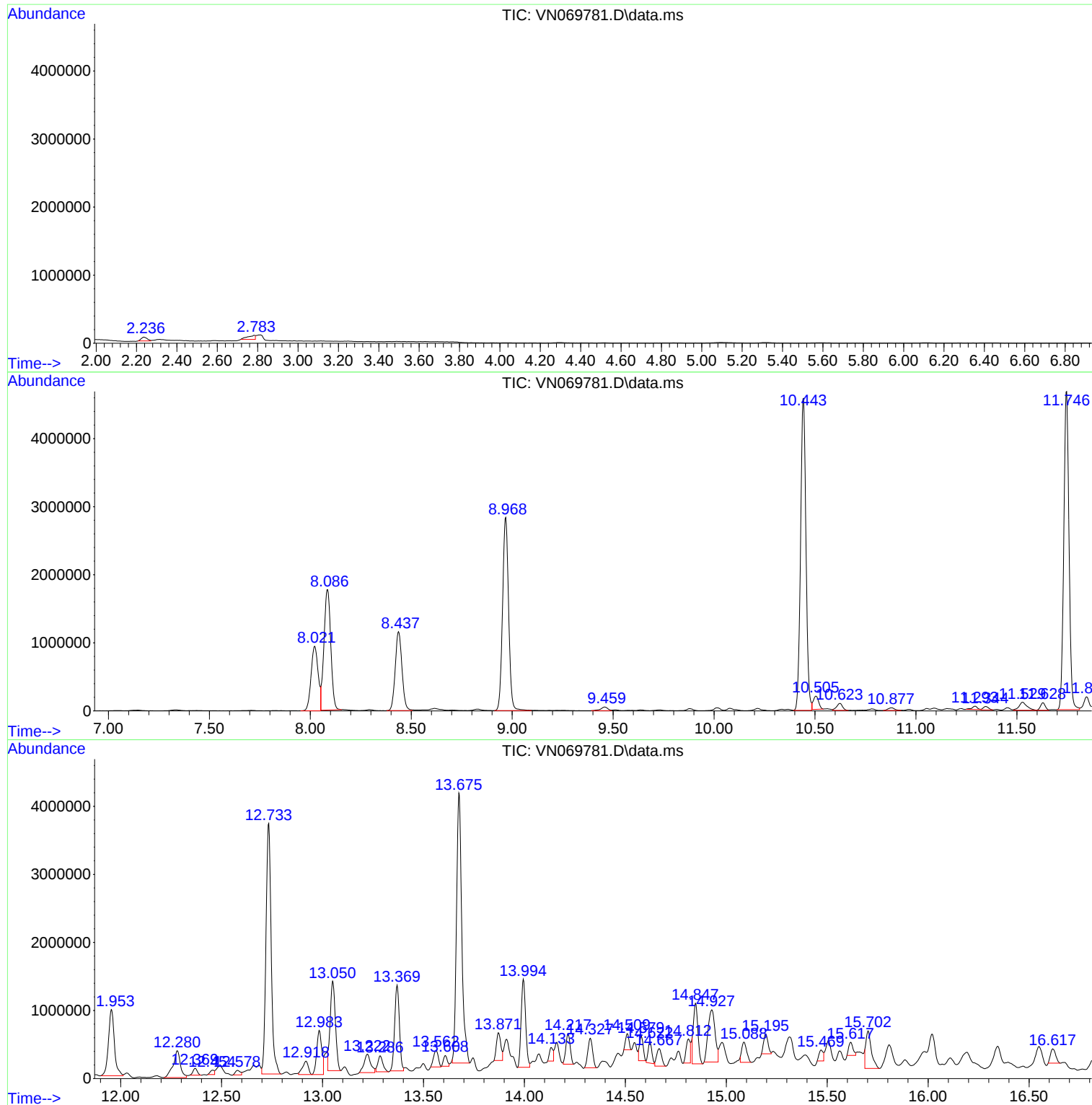
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Quant Title : SW846 8260

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



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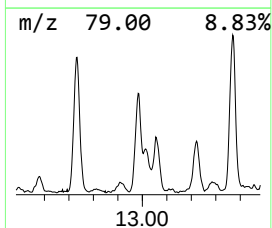
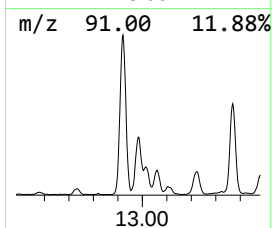
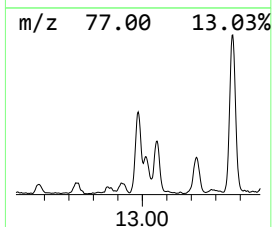
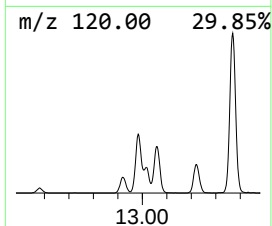
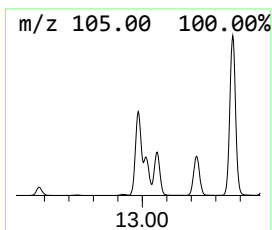
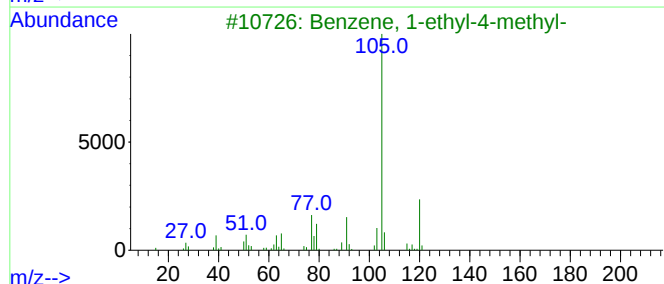
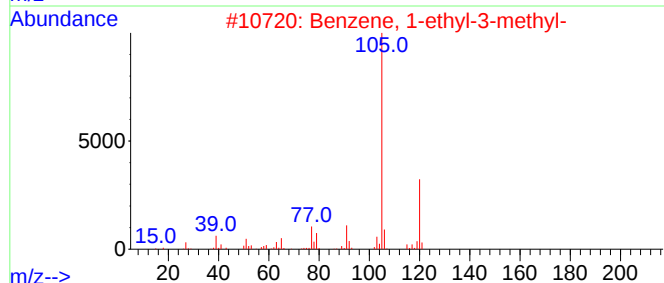
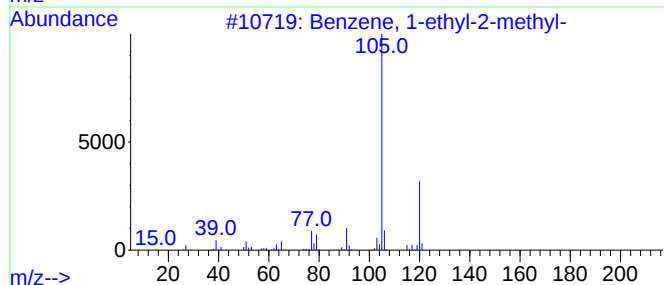
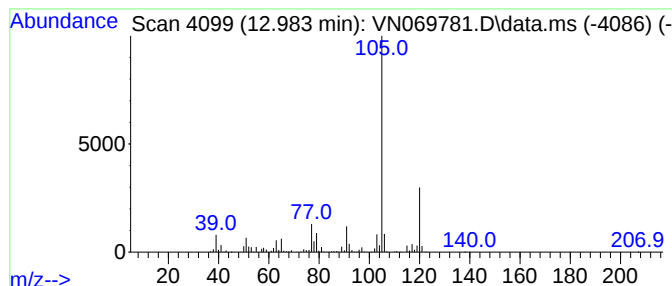
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	7.79 ug/l	1120690	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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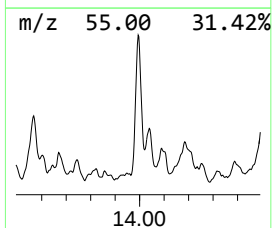
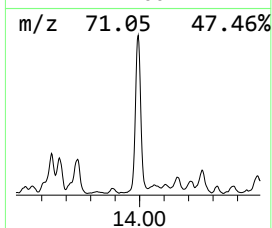
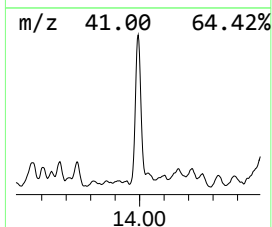
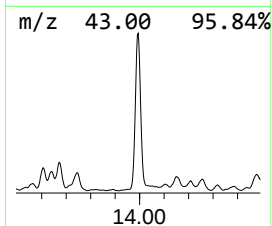
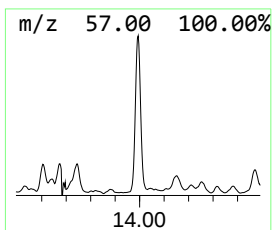
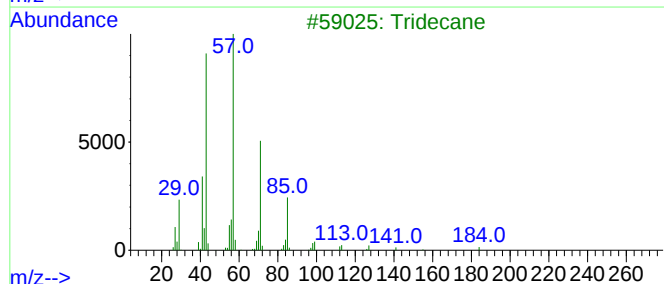
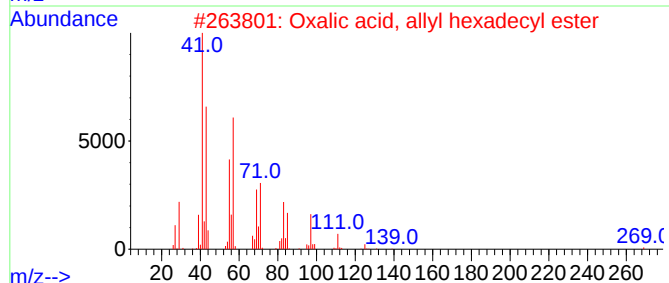
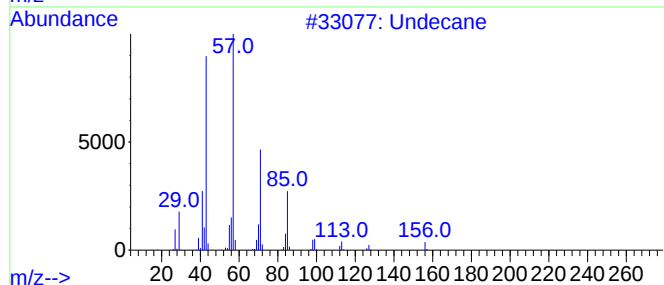
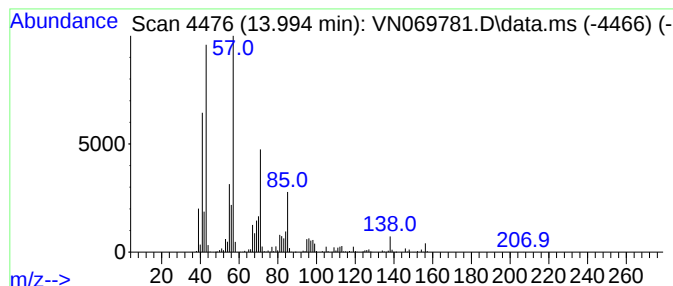
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 2 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	13.91 ug/l	2001810	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	87
2	Oxalic acid, allyl hexadecyl ester			354	C21H38O4	1000309-24-4	72
3	Tridecane			184	C13H28	000629-50-5	64
4	Carbonic acid, eicosyl vinyl ester			368	C23H44O3	1000382-54-3	64
5	Undecane, 2,3-dimethyl-			184	C13H28	017312-77-5	59



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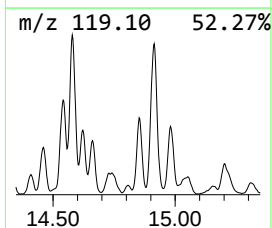
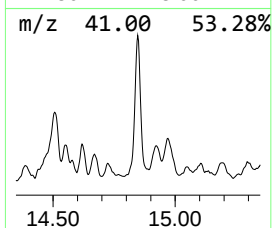
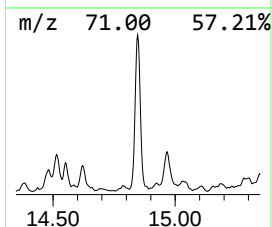
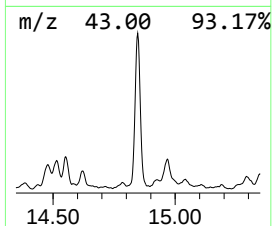
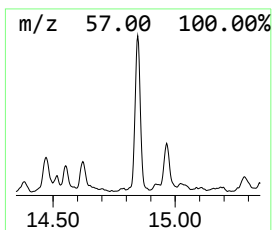
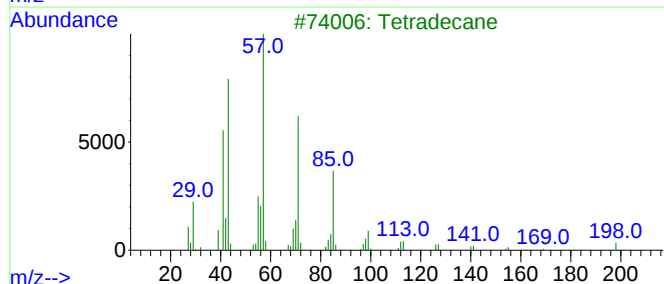
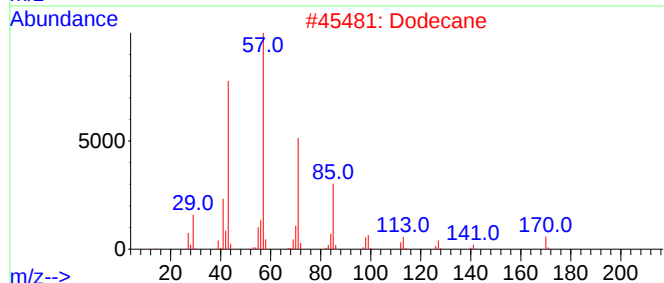
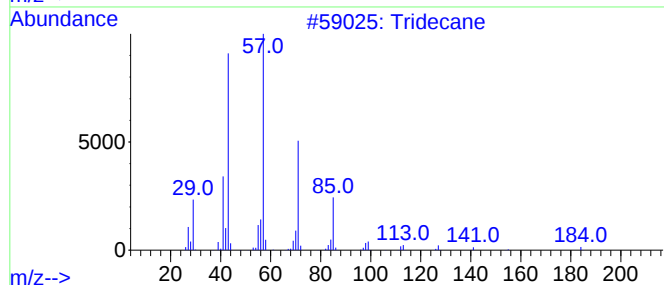
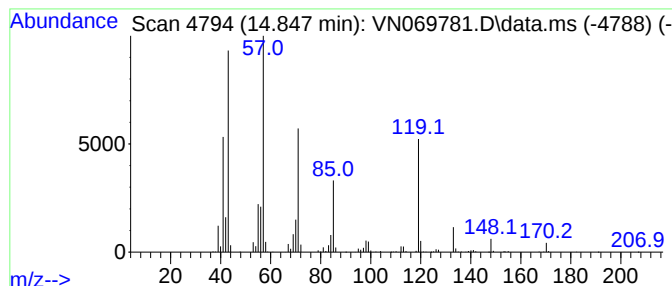
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Quant Title : SW846 8260

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

Peak Number 3 unknown14.847 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.847	9.48 ug/l	1363920	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	49
2			Dodecane	170	C12H26	000112-40-3	49
3			Tetradecane	198	C14H30	000629-59-4	49
4			Undecane	156	C11H24	001120-21-4	47
5			Hexadecane	226	C16H34	000544-76-3	43



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Instrument :
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ClientSampleId :
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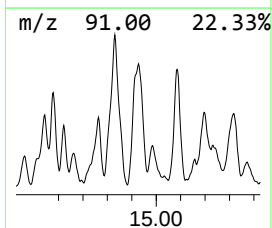
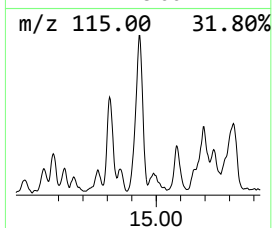
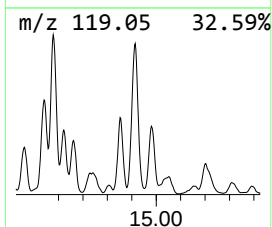
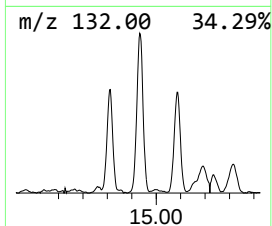
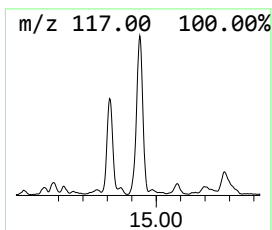
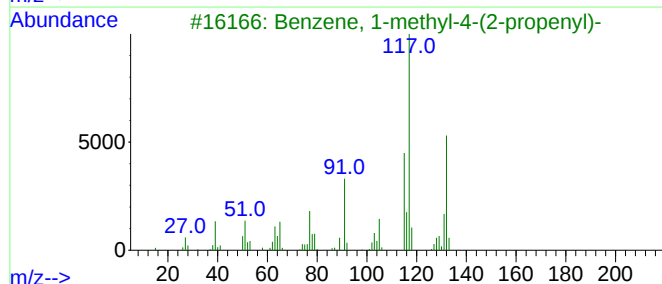
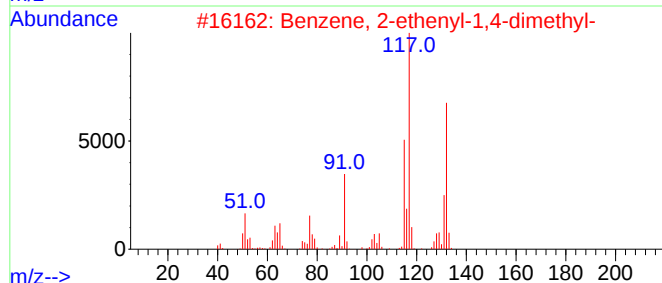
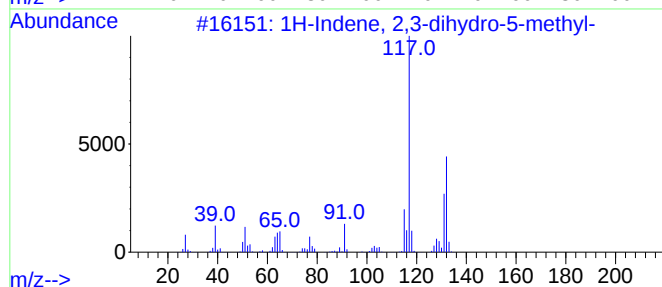
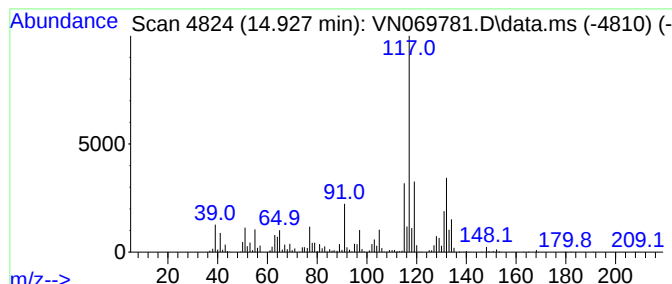
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Quant Title : SW846 8260

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

Peak Number 4 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	12.99 ug/l	1869140	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	92
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
4			2,4-Dimethylstyrene	132	C10H12	002234-20-0	87
5			3-Phenylbut-1-ene	132	C10H12	000934-10-1	76



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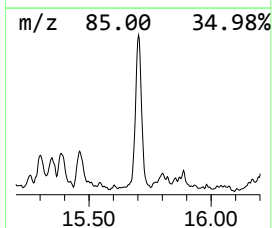
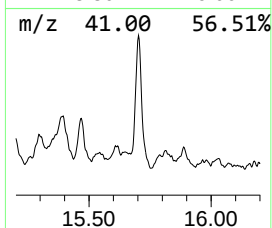
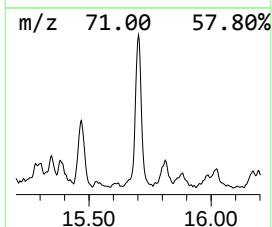
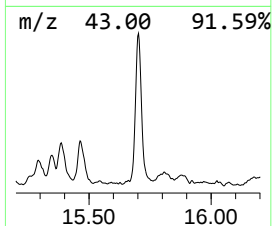
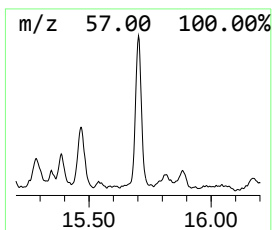
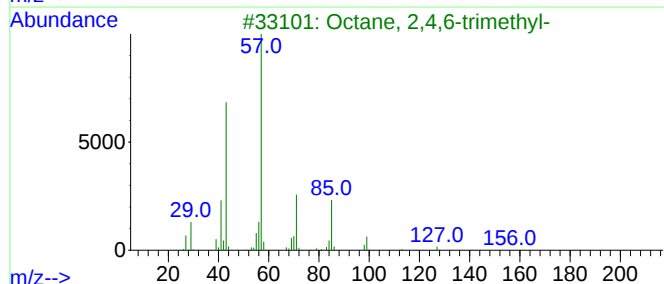
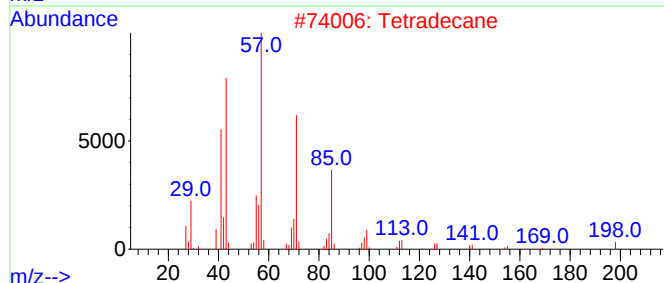
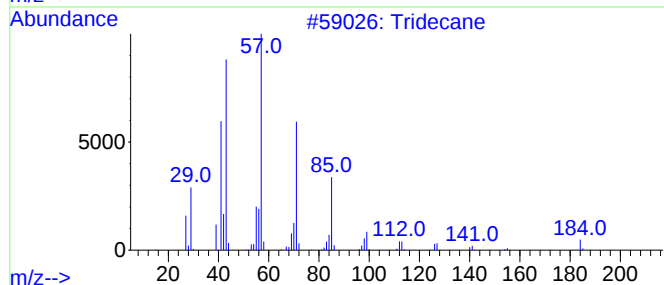
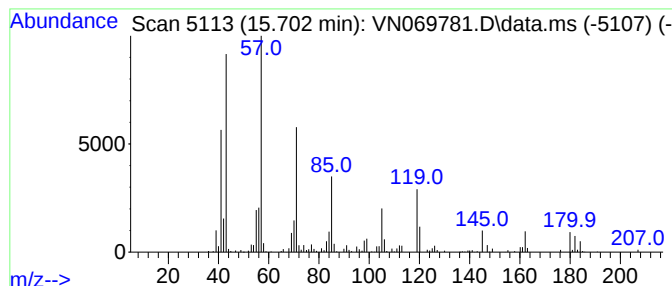
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 5 Tridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.702	7.17 ug/l	1031400	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	60
2			Tetradecane	198	C14H30	000629-59-4	38
3			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	38
4			Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	35
5			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120621\
Data File : VN069781.D
Acq On : 6 Dec 2021 14:10
Operator : JC/MD
Sample : M4866-01 10X
Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41679

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethy...	12.983	7.8	ug/l	1120690	4	13.678	7195070	50.0
Undecane	13.994	13.9	ug/l	2001810	4	13.678	7195070	50.0
unknown14.847	14.847	9.5	ug/l	1363920	4	13.678	7195070	50.0
1H-Indene, 2,3-...	14.927	13.0	ug/l	1869140	4	13.678	7195070	50.0
Tridecane	15.702	7.2	ug/l	1031400	4	13.678	7195070	50.0