LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PS-104

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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\82N012521W.M
Title : SW846 8260

Signal : TIC: VN065616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.550	1788	1807	1817	rBV	131991	343561	6.07%	0.405%
2	7.624	1818	1830	1846	rVB	266868	656688	11.60%	0.774%
3	7.836	1881	1896	1910	rBV3	25556	63685	1.12%	0.075%
4	7.987	1927	1943	1967	rBV	166213	385658	6.81%	0.455%
5	8.396	2056	2070	2090	rBV	51295	106748	1.88%	0.126%
6	8.547	2102	2117	2136	rBV	404033	836116	14.76%	0.986%
7	9.042	2249	2271	2285	rBV	132713	315454	5.57%	0.372%
8	9.695	2462	2474	2496	rVB2	88242	215017	3.80%	0.254%
9	9.836	2498	2518	2538	rVB	73882	180943	3.19%	0.213%
10	10.055	2571	2586	2598	rBV	760816	1469325	25.94%	1.733%
11	10.122	2599	2607	2618	rVV	277433	514157	9.08%	0.606%
12	10.251	2632	2647	2661	rVB2	313589	594353	10.49%	0.701%
13	10.399	2663	2693	2708	rVB2	81675	181602	3.21%	0.214%
14	10.499	2709	2724	2735	rBV2	99664	201787	3.56%	0.238%
15	10.595	2745	2754	2764	rVB3	38028	65803	1.16%	0.078%
16	10.688	2772	2783	2792	rBV2	72153	119897	2.12%	0.141%
17	10.791	2805	2815	2826	rBV	53751	102558	1.81%	0.121%
18	10.852	2826	2834	2839	rBV3	65334	100680	1.78%	0.119%
19	10.920	2848	2855	2863	rVB	167062	254556	4.49%	0.300%
20	10.974	2863	2872	2883	rVB2	151130	268005	4.73%	0.316%
21	11.090	2896	2908	2916	rBV5	87260	174918	3.09%	0.206%
22	11.171	2916	2933	2953	rVB5	399162	981163	17.32%	1.157%
23	11.270	2953	2964	2986	rBV	310460	581925	10.28%	0.686%
24	11.376	2986	2997	3017	rBV	524240	932209	16.46%	1.099%
25	11.479	3017	3029	3038	rBV	408839	774407	13.67%	0.913%
26	11.598	3046	3066	3081	rBV3	1876154	4883726	86.23%	5.759%
27	11.669	3082	3088	3098	rVB2	204357	340636	6.01%	0.402%
28	11.820	3128	3135	3143	rVB5	51688	80362	1.42%	0.095%
29	11.917	3143	3165	3181	rBV2	935240	2386474	42.14%	2.814%
30	12.016	3188	3196	3203	rBV	214952	302684	5.34%	0.357%
31	12.090	3211	3219	3224	rBV2	189979	305863	5.40%	0.361%
32	12.135	3225	3233	3250	rVB6	426137	892216	15.75%	1.052%
33	12.219	3252	3259	3266	rBV2	136648	216819	3.83%	0.256%
34	12.309	3282	3287	3291	rBV	137674	151061	2.67%	0.178%
35	12.373	3300	3307	3314	rVB	330715	465299	8.22%	0.549%
36	12.418	3314	3321	3330	rVB2	308953	413741	7.31%	0.488%

LSC Area Percent Report

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ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PS-104

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Title : SW846 8260

37	12.560	3350	3365	3373	rVB	452699	952560	16.82%	1.123%
38	12.624	3374	3385	3392	rBV	1805982	3081428	54.41%	3.634%
39	12.701	3401	3409	3419	rVB2	2986782	4677027	82.58%	5.516%
40	12.749	3419	3424	3434	rVB2	276623	422942	7.47%	0.499%
41	12.862	3446	3459	3468	rBV	841990	1577864	27.86%	1.861%
42	12.933	3474	3481	3493	rVB2	465997	804068	14.20%	0.948%
43	13.010	3493	3505	3516	rBV	3499882	5663339	100.00%	6.679%
44	13.138	3533	3545	3553	rVB5	312112	599520	10.59%	0.707%
45	13.206	3554	3566	3575	rBV3	676042	1303960	23.02%	1.538%
46	13.257	3576	3582	3588	rVV2	301876	423752	7.48%	0.500%
47	13.344	3589	3609	3618	rVB2	1074780	2680326	47.33%	3.161%
48	13.396	3619	3625	3631	rBV2	150521	196953	3.48%	0.232%
49	13.511	3646	3661	3668	rBV	1364161	2448335	43.23%	2.887%
50	13.556	3668	3675	3690	rVB4	1127430	2269266	40.07%	2.676%
51	13.643	3690	3702	3711	rBV3	1580442	2623204	46.32%	3.093%
52	13.711	3716	3723	3733	rVB	562404	855310	15.10%	1.009%
53	13.772	3734	3742	3746	rVV	645594	916409	16.18%	1.081%
54	13.801	3747	3751	3760	rVV	771893	1088434	19.22%	1.284%
55	13.859	3761	3769	3778	rVB	982268	1474855	26.04%	1.739%
56	13.910	3780	3785	3792	rVB2	149775	201922	3.57%	0.238%
57	13.965	3792	3802	3812	rVB	1106440	1802551	31.83%	2.126%
58	14.042	3813	3826	3833	rBV6	210913	547919	9.67%	0.646%
59	14.138	3849	3856	3862	rBV9	323254	549324	9.70%	0.648%
60	14.177	3864	3868	3874	rVV	465206	688254	12.15%	0.812%
61	14.219	3875	3881	3888	rVB	889729	1283587	22.66%	1.514%
62	14.264	3888	3895	3901	rBV2	491569	667044	11.78%	0.787%
63	14.302	3902	3907	3915	rVB2	436654	568389	10.04%	0.670%
64	14.402	3934	3938	3944	rVB2	350452	409848	7.24%	0.483%
65	14.447	3945	3952	3959	rVV2	567407	1002929	17.71%	1.183%
66	14.492	3960	3966	3975	rVB	1255652	1866511	32.96%	2.201%
67	14.556	3975	3986	3998	rBV4	1597904	3683628	65.04%	4.344%
68	14.617	3999	4005	4015	rVB3	418574	681830	12.04%	0.804%
69	14.711	4025	4034	4045	rVB	899787	1446590	25.54%	1.706%
70	14.785	4051	4057	4059	rBV4	168340	190800	3.37%	0.225%
71	14.820	4061	4068	4074	rVV4	485897	765096	13.51%	0.902%
72	14.926	4092	4101	4113	rVB3	610260	1214851	21.45%	1.433%
73	15.080	4141	4149	4154	rBV5	262561	452820	8.00%	0.534%
74	15.154	4165	4172	4180	rBV2	495285	757786	13.38%	0.894%
75	15.209	4181	4189	4208	rVV5	579690	1716680	30.31%	2.024%
76	15.296	4209	4216	4230	rVB4	716493	1271664	22.45%	1.500%

LSC Area Percent Report

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Instrument : MSVOA_N
ClientSampleId : PS-104

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Integrator: RTE
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Sampling : 1 Min Area: 1 % of largest Peak
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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Title : SW846 8260

77	15.379	4231	4242	4256	rBV4	447939	1075406	18.99%	1.268%
78	15.576	4295	4303	4316	rVB	1132959	2031217	35.87%	2.395%
79	15.730	4341	4351	4374	rVB6	367035	1085264	19.16%	1.280%
80	15.868	4382	4394	4405	rBV2	721429	1492152	26.35%	1.760%
81	16.058	4443	4453	4463	rVB3	681683	1287205	22.73%	1.518%
82	16.116	4464	4471	4485	rBV5	319378	624630	11.03%	0.737%
83	16.309	4521	4531	4541	rBV8	189881	512217	9.04%	0.604%

Sum of corrected areas: 84797762

LSC Report - Integrated Chromatogram

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Sample : M1216-02 20X
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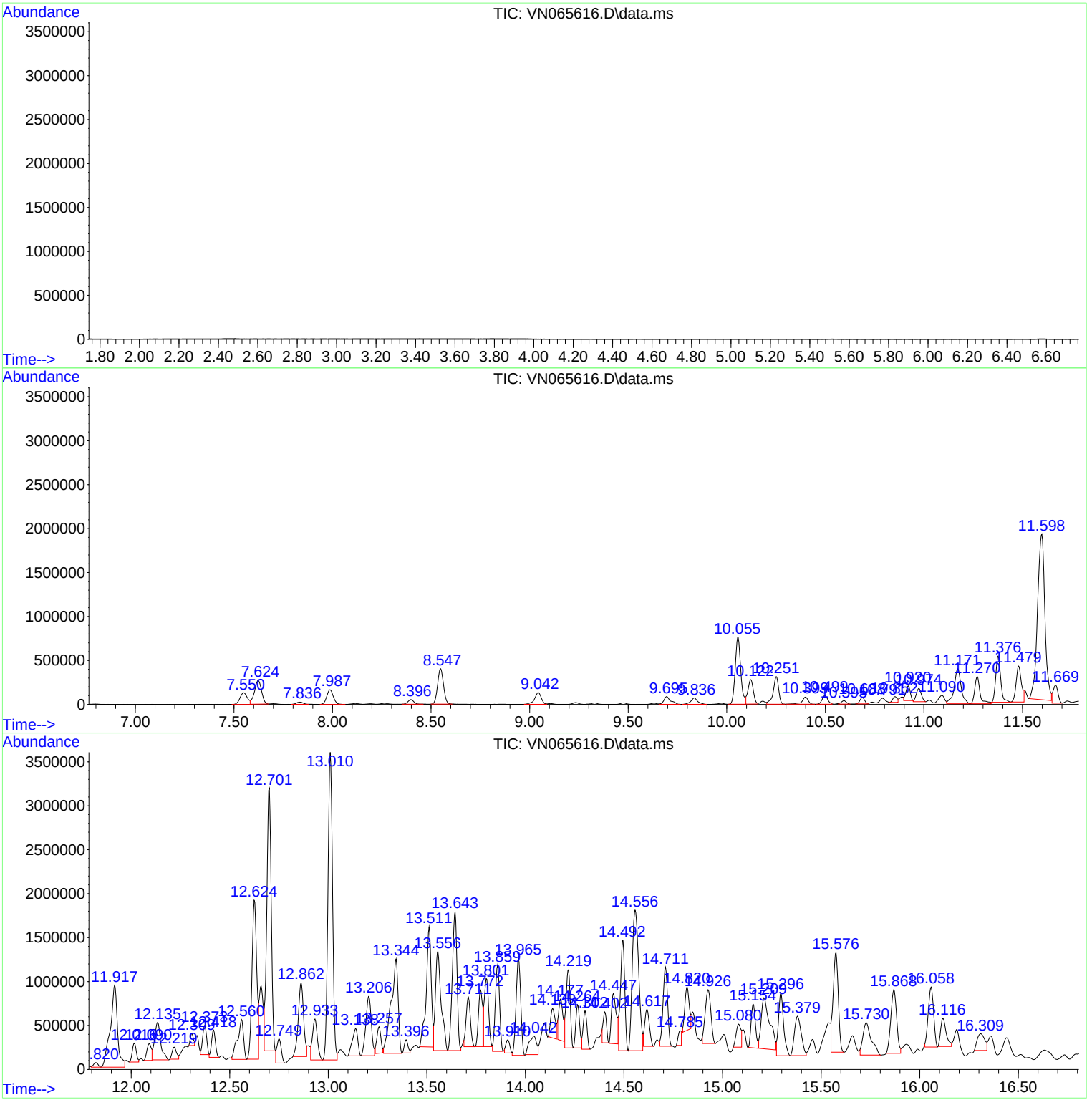
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

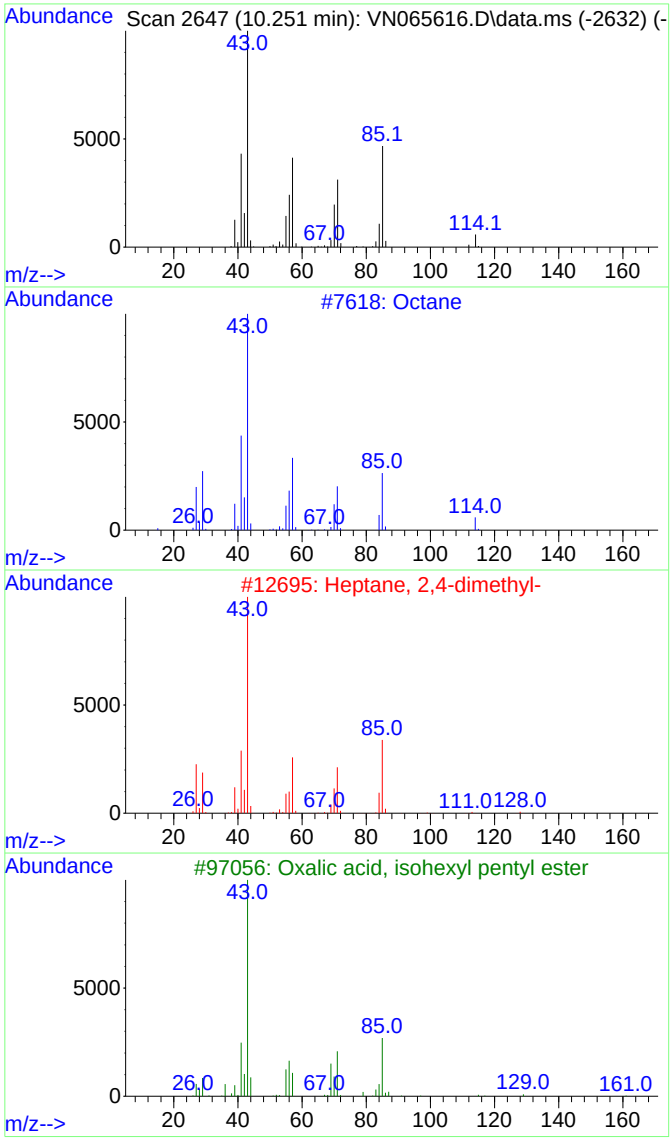
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

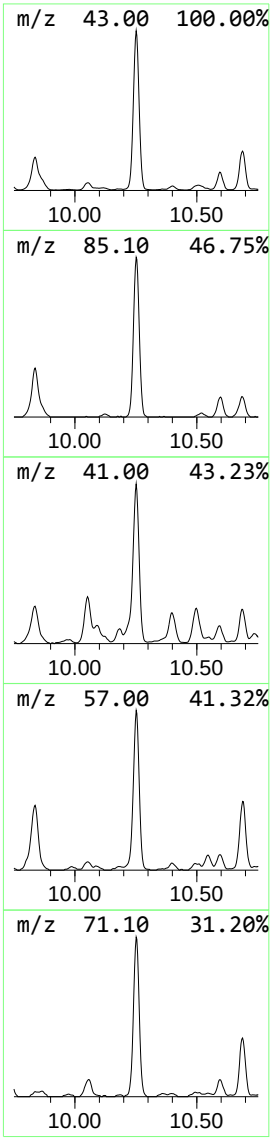
****

Peak Number 1 Octane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.251	31.88 ug/l	594353	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane	114	C8H18	000111-65-9	94
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3	Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	72
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	64
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	59





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Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

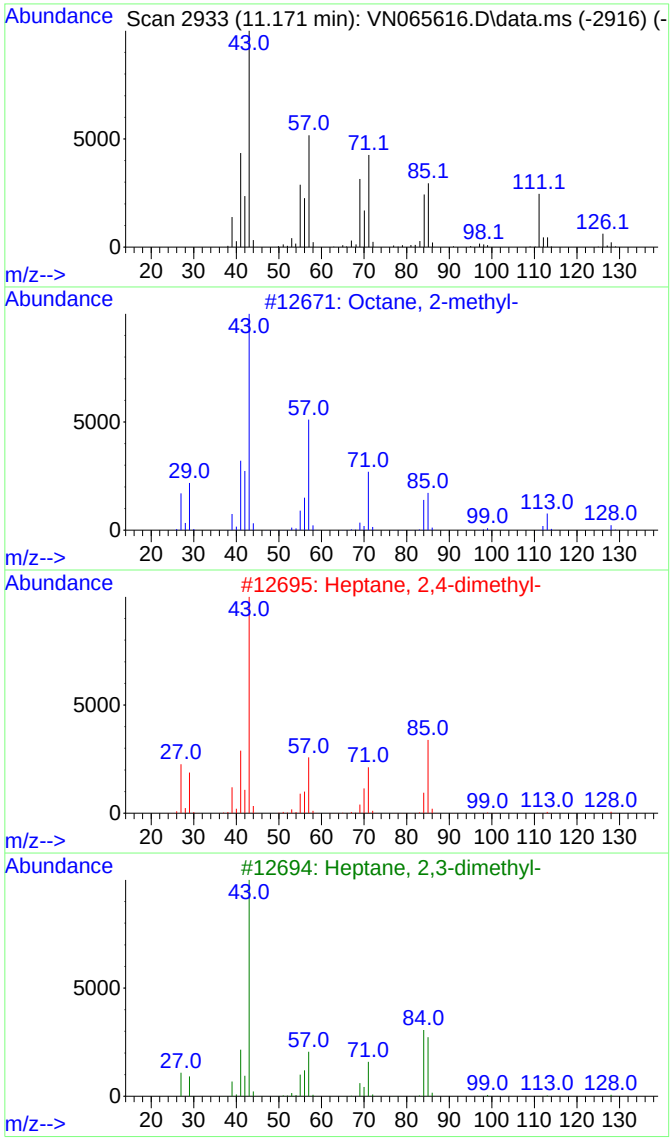
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

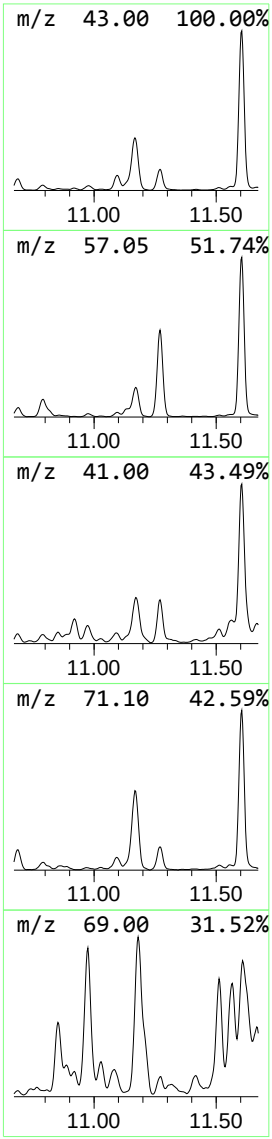
****

Peak Number 2 Octane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.171	52.63 ug/l	981163	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	50
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	47
3	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	43
4	Octane, 4-methyl-	128	C9H20	002216-34-4	43
5	Trichloroacetic acid, 4-methylpe...	246	C8H13Cl3O2	1000282-35-2	38





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Instrument :
MSVOA_N
ClientSampleId :
PS-104

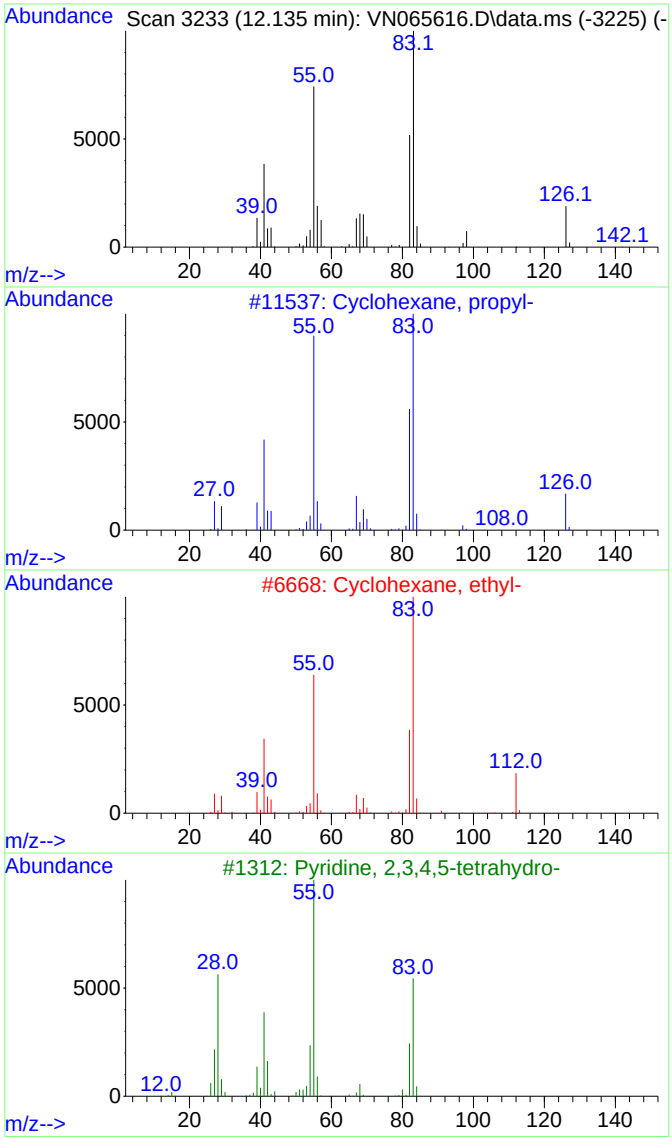
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

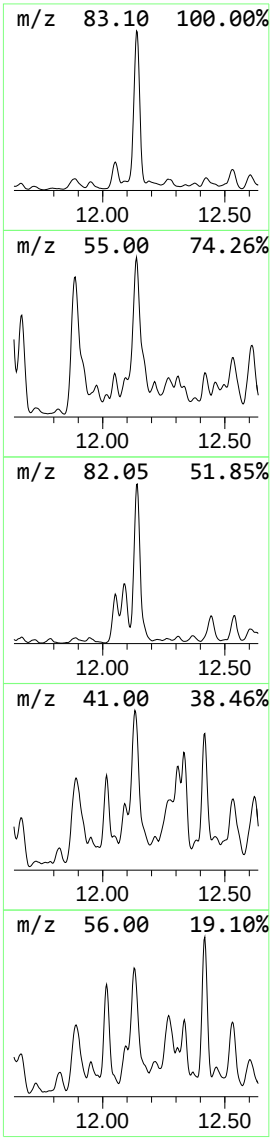
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexane, propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.135	47.85 ug/l	892216	Chlorobenzene-d5	11.376

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	90
2	Cyclohexane, ethyl-	112	C8H16	001678-91-7	72
3	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	59
4	Cyclohexane, decyl-	224	C16H32	001795-16-0	59
5	Ethanone, 1-(1-methylcyclopentyl)-	126	C8H14O	013388-93-7	53





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Instrument :
MSVOA_N
ClientSampleId :
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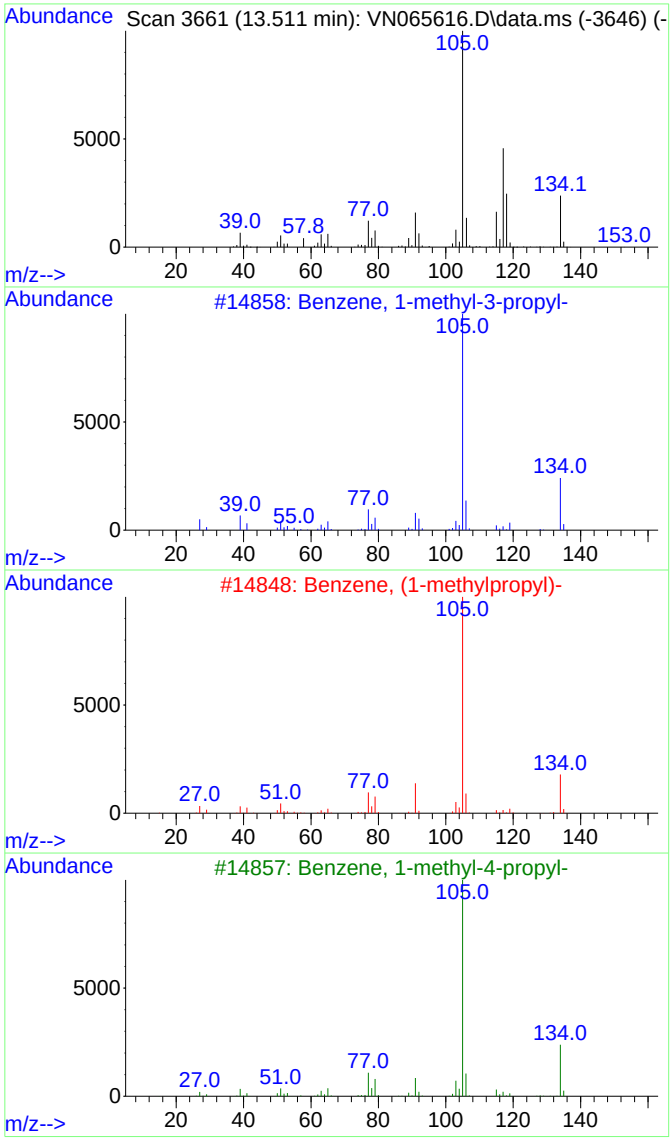
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

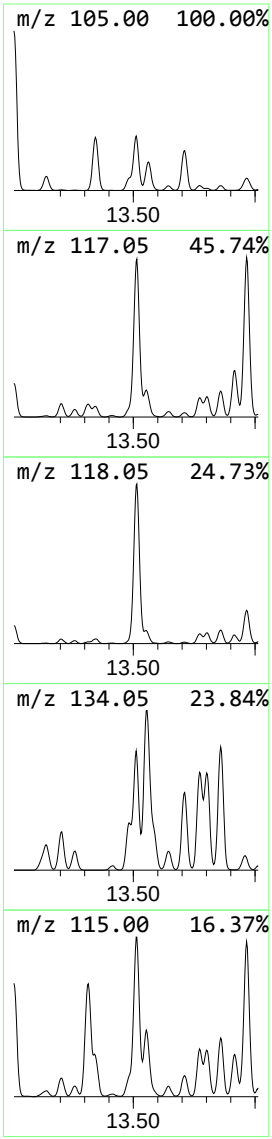
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-methyl-3-propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.511	45.67 ug/l	2448340	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	50
2	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	50
3	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	46
4	Benzene, 1-methyl-2-propyl-	134	C10H14	001074-17-5	45
5	2-Indanol	134	C9H10O	004254-29-9	43





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

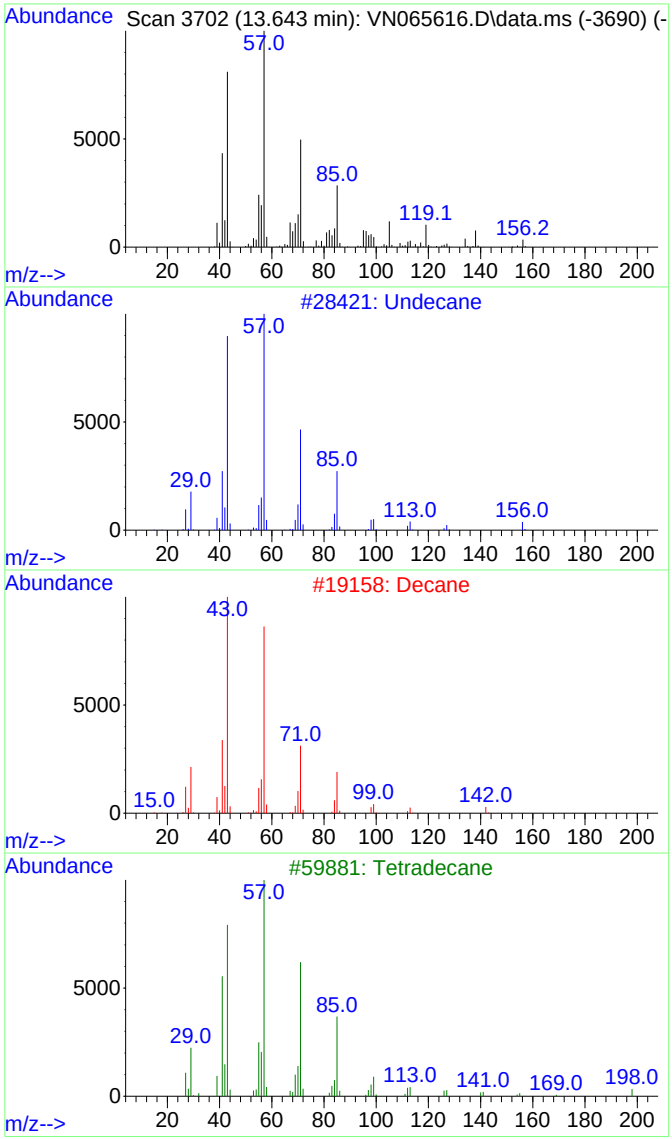
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

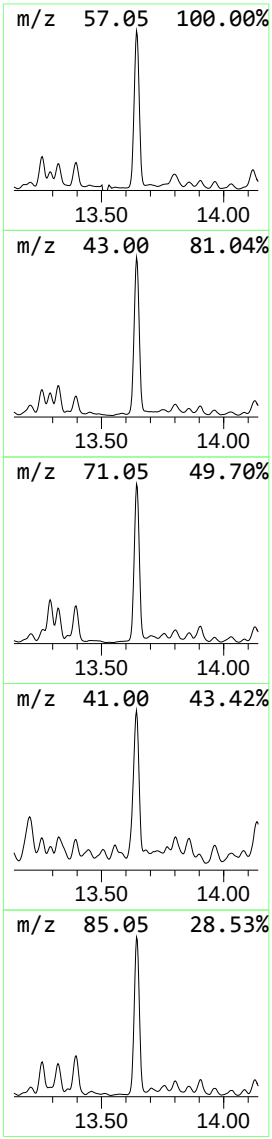
****

Peak Number 5 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.643	48.93 ug/l	2623200	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	89
2	Decane	142	C10H22	000124-18-5	64
3	Tetradecane	198	C14H30	000629-59-4	64
4	Octacosane	394	C28H58	000630-02-4	59
5	Hexadecane	226	C16H34	000544-76-3	52





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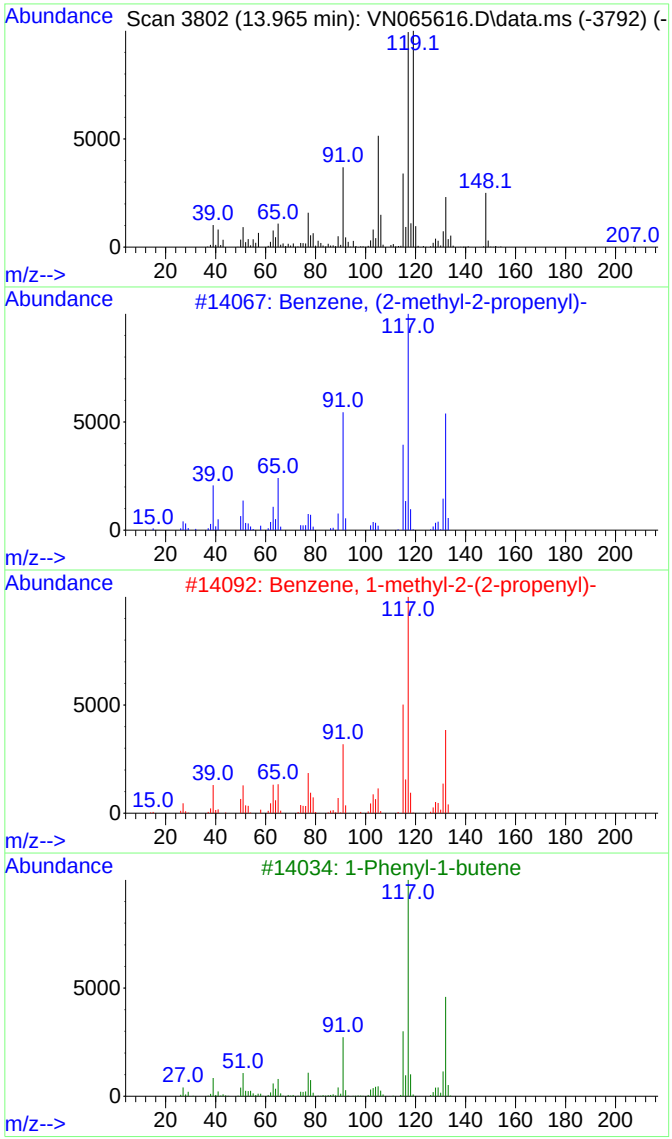
Quant Title : SW846 8260

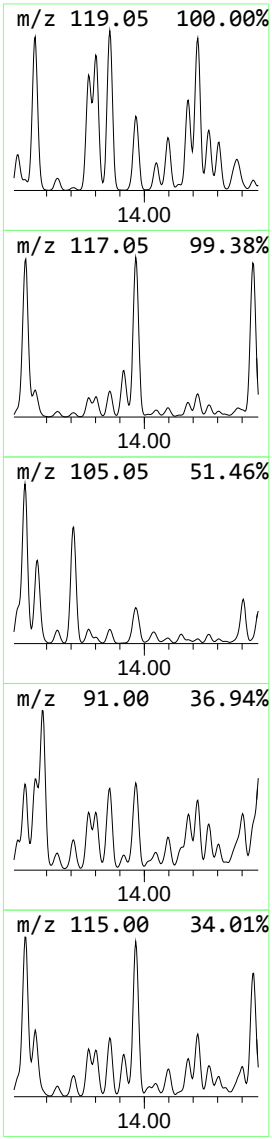
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, (2-methyl-2-propen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	33.63 ug/l	1802550	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	86
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	64
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64
5	Indan, 1-methyl-	132	C10H12	000767-58-8	50





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Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

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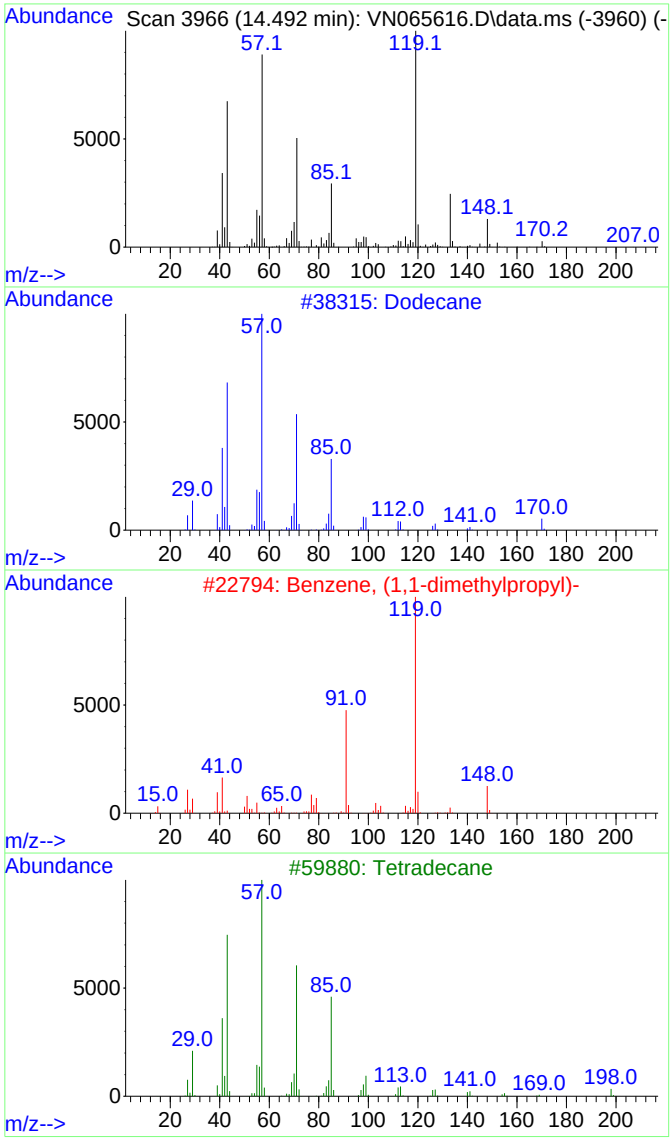
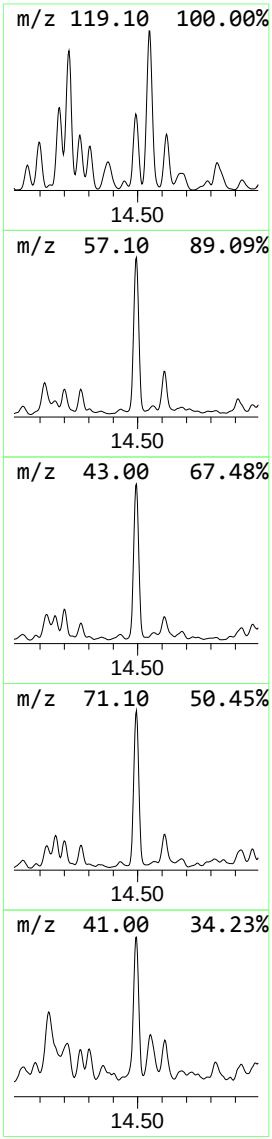
Peak Number 7 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.492	34.82 ug/l	1866510	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	81
2	Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	38
3	Tetradecane	198	C14H30	000629-59-4	30
4	Hexadecane	226	C16H34	000544-76-3	30
5	Tridecane	184	C13H28	000629-50-5	30





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Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

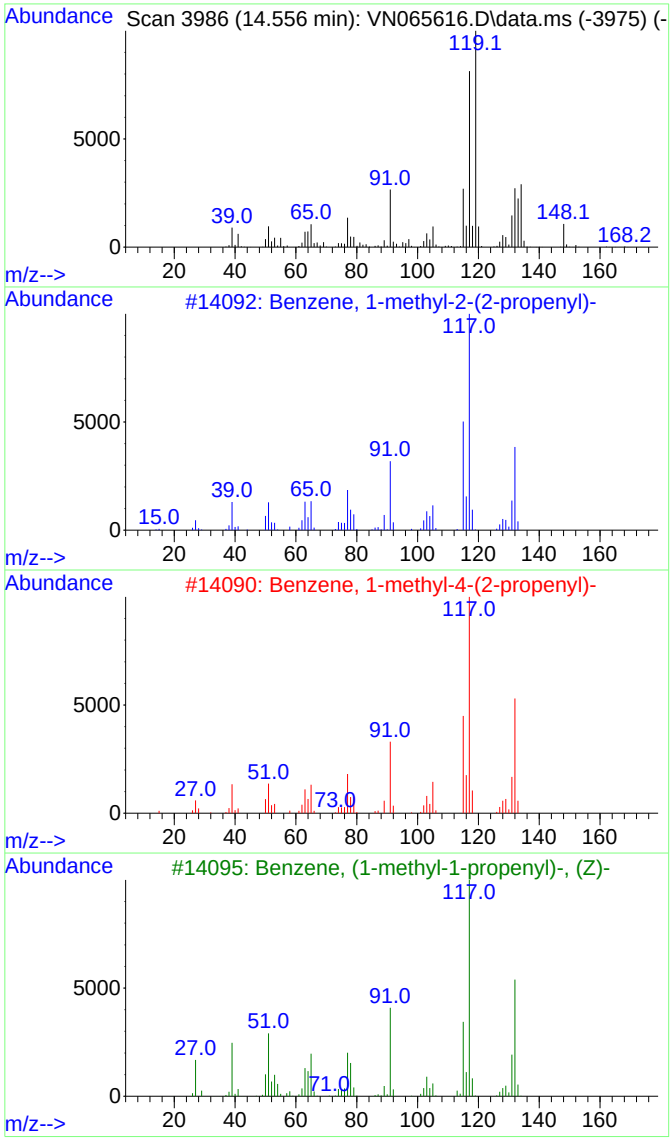
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

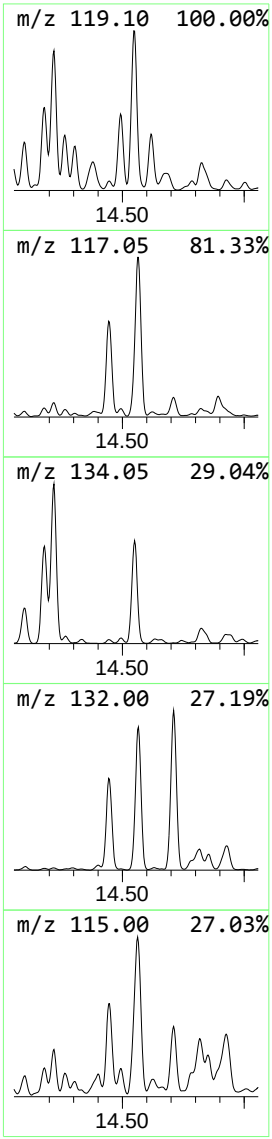
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-methyl-2-(2-prop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.556	68.72 ug/l	3683630	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
2	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	74
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	64
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	64
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64





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Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

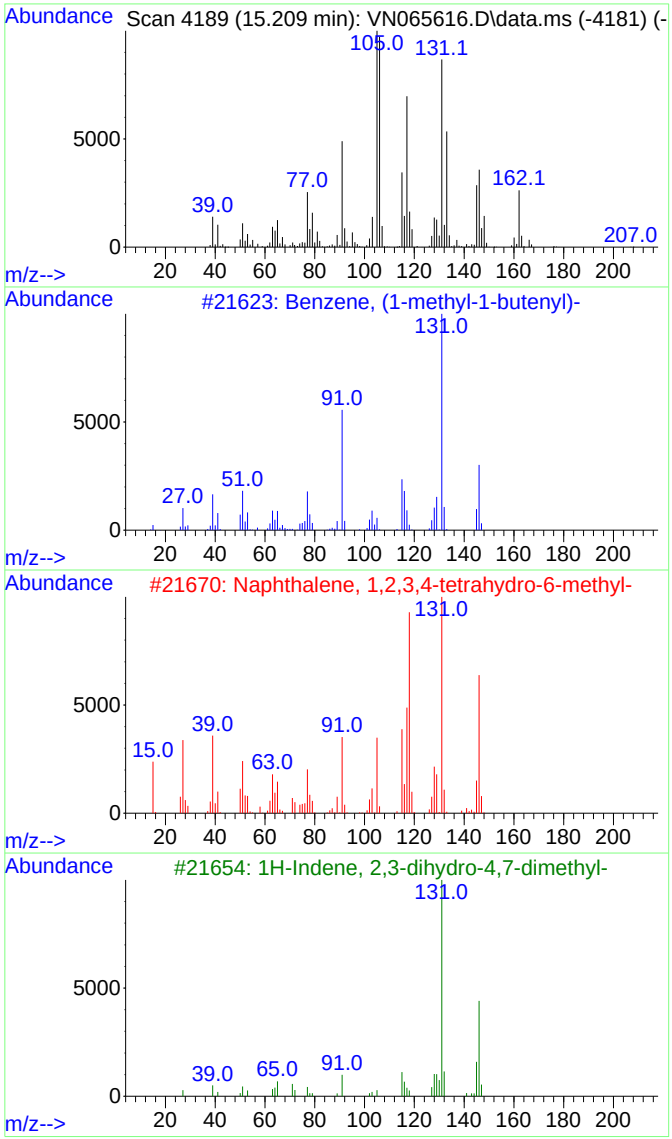
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

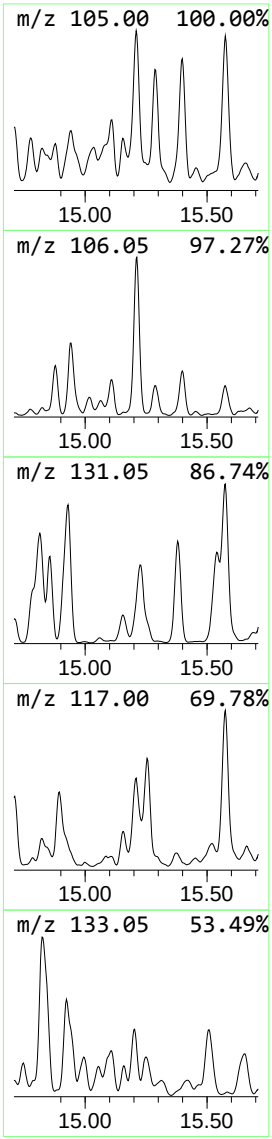
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, (1-methyl-1-butenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.209	32.02 ug/l	1716680	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methyl-1-butenyl)-	146	C11H14	053172-84-2	80
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	50
3	1H-Indene, 2,3-dihydro-4,7-dimet...	146	C11H14	006682-71-9	42
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	42
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PS-104

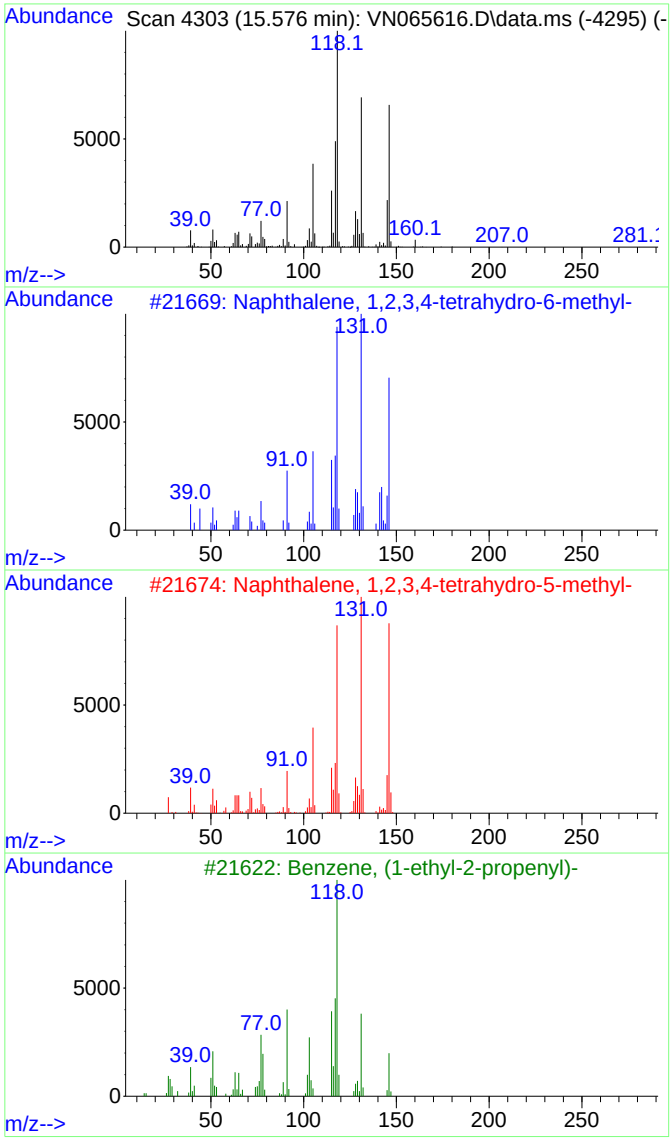
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

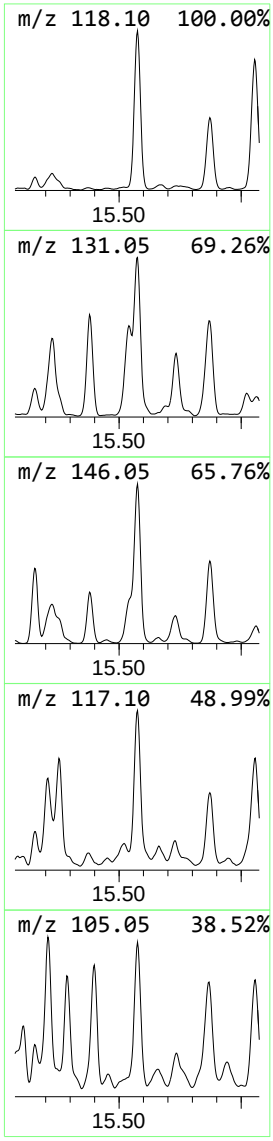
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Naphthalene, 1,2,3,4-tetrah... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.576	37.89 ug/l	2031220	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001680-51-9	83
2	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	83
3	Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	72
4	2,3,4,5,6,7-Hexahydro-1H-cyclope...	146	C11H14	1000189-31-0	58
5	2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN012621\
Data File : VN065616.D
Acq On : 26 Jan 2021 20:07
Operator : JC/MD
Sample : M1216-02 20X
Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : PS-104

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Octane	10.251	31.9	ug/l	594353	3	11.376	932209	50.0
Octane, 2-methyl-	11.171	52.6	ug/l	981163	3	11.376	932209	50.0
Cyclohexane, pr...	12.135	47.9	ug/l	892216	3	11.376	932209	50.0
Benzene, 1-meth...	13.511	45.7	ug/l	2448340	4	13.312	2680330	50.0
Undecane	13.643	48.9	ug/l	2623200	4	13.312	2680330	50.0
Benzene, (2-met...	13.965	33.6	ug/l	1802550	4	13.312	2680330	50.0
Dodecane	14.492	34.8	ug/l	1866510	4	13.312	2680330	50.0
Benzene, 1-meth...	14.556	68.7	ug/l	3683630	4	13.312	2680330	50.0
Benzene, (1-met...	15.209	32.0	ug/l	1716680	4	13.312	2680330	50.0
Naphthalene, 1,...	15.576	37.9	ug/l	2031220	4	13.312	2680330	50.0