LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 124-SB-1

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\82N042121W.M
Title : SW846 8260

Signal : TIC: VN066740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.763	372	388	407	rBV2	99933	202336	7.38%	0.503%
2	3.091	496	510	530	rVB3	28285	62170	2.27%	0.155%
3	3.740	730	752	772	rBV4	15050	47733	1.74%	0.119%
4	4.512	991	1040	1096	rBV2	287568	1188624	43.33%	2.956%
5	4.968	1177	1210	1246	rBV2	201420	717891	26.17%	1.785%
6	5.480	1379	1401	1429	rBV5	25694	82599	3.01%	0.205%
7	5.842	1511	1536	1560	rBV3	17076	52038	1.90%	0.129%
8	5.985	1567	1589	1613	rBV5	14259	47791	1.74%	0.119%
9	6.277	1673	1698	1726	rBV8	29708	106712	3.89%	0.265%
10	6.438	1734	1758	1776	rBV2	70671	221992	8.09%	0.552%
11	6.542	1776	1797	1821	rVB2	190814	578660	21.10%	1.439%
12	7.250	2040	2061	2068	rBV4	15005	38294	1.40%	0.095%
13	7.312	2071	2084	2106	rVB4	39408	110758	4.04%	0.275%
14	7.519	2130	2161	2164	rBV2	196006	418407	15.25%	1.041%
15	7.580	2168	2184	2203	rVV5	549646	2004841	73.09%	4.986%
16	7.671	2204	2218	2245	rVV2	227282	621766	22.67%	1.546%
17	7.806	2246	2268	2305	rVV	575908	1496672	54.56%	3.722%
18	7.956	2306	2324	2352	rVV2	212179	526885	19.21%	1.310%
19	8.087	2353	2373	2381	rVV3	234457	562217	20.50%	1.398%
20	8.144	2384	2394	2415	rVV3	396749	1212979	44.22%	3.017%
21	8.235	2416	2428	2454	rVV2	171111	437225	15.94%	1.087%
22	8.342	2455	2468	2495	rVB6	24545	80858	2.95%	0.201%
23	8.516	2512	2533	2561	rBV	636753	1497377	54.59%	3.724%
24	8.680	2583	2594	2608	rVB3	30147	55794	2.03%	0.139%
25	8.755	2608	2622	2631	rBV2	53997	112154	4.09%	0.279%
26	9.015	2685	2719	2734	rBV2	756219	2057815	75.02%	5.118%
27	9.080	2734	2743	2761	rVB2	193000	380271	13.86%	0.946%
28	9.206	2778	2790	2805	rVV	144712	288102	10.50%	0.717%
29	9.302	2805	2826	2843	rVV4	150421	360000	13.12%	0.895%
30	9.452	2868	2882	2907	rBV4	263897	542365	19.77%	1.349%
31	9.554	2909	2920	2926	rBV2	98922	177729	6.48%	0.442%
32	9.600	2928	2937	2949	rVB5	197037	370280	13.50%	0.921%
33	9.670	2950	2963	2969	rBV	270077	483414	17.62%	1.202%
34	9.809	2992	3015	3041	rBV	495788	1248752	45.52%	3.106%
35	9.908	3041	3052	3059	rBV3	53777	101335	3.69%	0.252%
36	9.959	3061	3071	3082	rVB4	99562	191444	6.98%	0.476%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 124-SB-1

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\82N042121W.M
Title : SW846 8260

37	10.026	3082	3096	3125	rVB3	1262693	2743009	100.00%	6.822%
38	10.155	3127	3144	3151	rBV	119691	237793	8.67%	0.591%
39	10.198	3152	3160	3165	rBV3	115396	182721	6.66%	0.454%
40	10.332	3202	3210	3215	rVV4	56182	79029	2.88%	0.197%
41	10.372	3216	3225	3245	rVB	199380	353225	12.88%	0.878%
42	10.466	3246	3260	3276	rBV6	278140	638701	23.28%	1.588%
43	10.568	3289	3298	3310	rVB4	127354	218603	7.97%	0.544%
44	10.662	3310	3333	3344	rBV	242635	444870	16.22%	1.106%
45	10.764	3345	3371	3385	rBV	229903	557288	20.32%	1.386%
46	10.825	3387	3394	3400	rBV7	69210	98829	3.60%	0.246%
47	10.893	3412	3419	3428	rVB	236402	335699	12.24%	0.835%
48	10.946	3429	3439	3452	rVB2	301648	524981	19.14%	1.306%
49	11.003	3454	3460	3470	rVB6	76565	106547	3.88%	0.265%
50	11.064	3472	3483	3492	rBV6	149426	252336	9.20%	0.628%
51	11.142	3494	3512	3537	rVB5	488097	1326325	48.35%	3.299%
52	11.244	3537	3550	3576	rBV	488860	963188	35.11%	2.395%
53	11.348	3577	3589	3611	rBV	735222	1375015	50.13%	3.420%
54	11.453	3618	3628	3648	rVB	266951	564711	20.59%	1.404%
55	11.531	3649	3657	3669	rVB7	111601	203592	7.42%	0.506%
56	11.598	3672	3682	3692	rBV2	182653	322602	11.76%	0.802%
57	11.700	3711	3720	3729	rBV6	38230	68631	2.50%	0.171%
58	11.753	3732	3740	3748	rVV5	40666	63449	2.31%	0.158%
59	11.799	3749	3757	3767	rBV5	73575	114061	4.16%	0.284%
60	11.869	3768	3783	3798	rBV6	222084	576511	21.02%	1.434%
61	11.989	3820	3828	3843	rVB	242584	333599	12.16%	0.830%
62	12.062	3846	3855	3863	rVV3	194534	312355	11.39%	0.777%
63	12.105	3864	3871	3883	rVB5	204763	350752	12.79%	0.872%
64	12.346	3953	3961	3972	rVB	402720	593462	21.64%	1.476%
65	12.504	4014	4020	4023	rBV3	70565	82185	3.00%	0.204%
66	12.537	4025	4032	4043	rVB	282002	409406	14.93%	1.018%
67	12.837	4135	4144	4153	rBV	227163	346221	12.62%	0.861%
68	12.907	4164	4170	4185	rVB3	240712	373801	13.63%	0.930%
69	13.035	4212	4218	4229	rVB2	94897	140696	5.13%	0.350%
70	13.094	4232	4240	4243	rBV4	99916	130485	4.76%	0.325%
71	13.229	4284	4290	4297	rBV2	110049	129813	4.73%	0.323%
72	13.290	4299	4313	4334	rVB	709661	1389734	50.66%	3.456%
73	13.457	4367	4375	4380	rBV	160262	223805	8.16%	0.557%
74	13.542	4399	4407	4409	rBV2	71211	85255	3.11%	0.212%
75	13.832	4505	4515	4527	rBV	519429	788119	28.73%	1.960%
76	13.937	4544	4554	4568	rVB	378179	596710	21.75%	1.484%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 124-SB-1

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\82N042121W.M
Title : SW846 8260

77	14.151	4628	4634	4655	rVB	307790	566721	20.66%	1.409%
78	14.240	4658	4667	4675	rBV3	146582	225199	8.21%	0.560%
79	14.419	4725	4734	4744	rBV2	193596	311957	11.37%	0.776%
80	14.468	4747	4752	4761	rVB4	113670	143882	5.25%	0.358%
81	14.532	4762	4776	4789	rBV4	460576	958606	34.95%	2.384%
82	14.792	4866	4873	4882	rVB3	160563	209114	7.62%	0.520%
83	14.899	4904	4913	4928	rVB2	174623	333284	12.15%	0.829%
84	15.350	5072	5081	5101	rVB	75786	135460	4.94%	0.337%

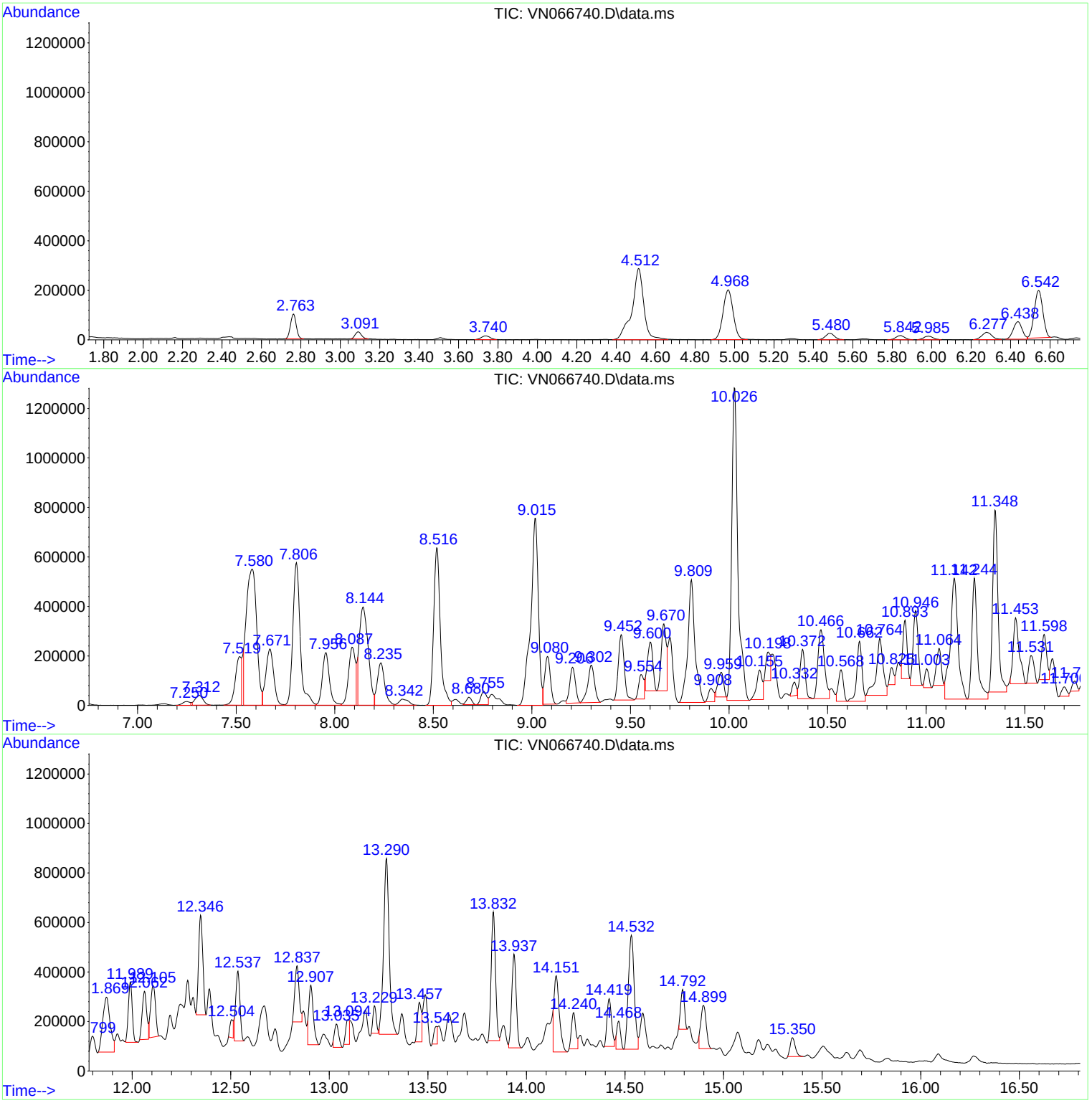
Sum of corrected areas: 40208617

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

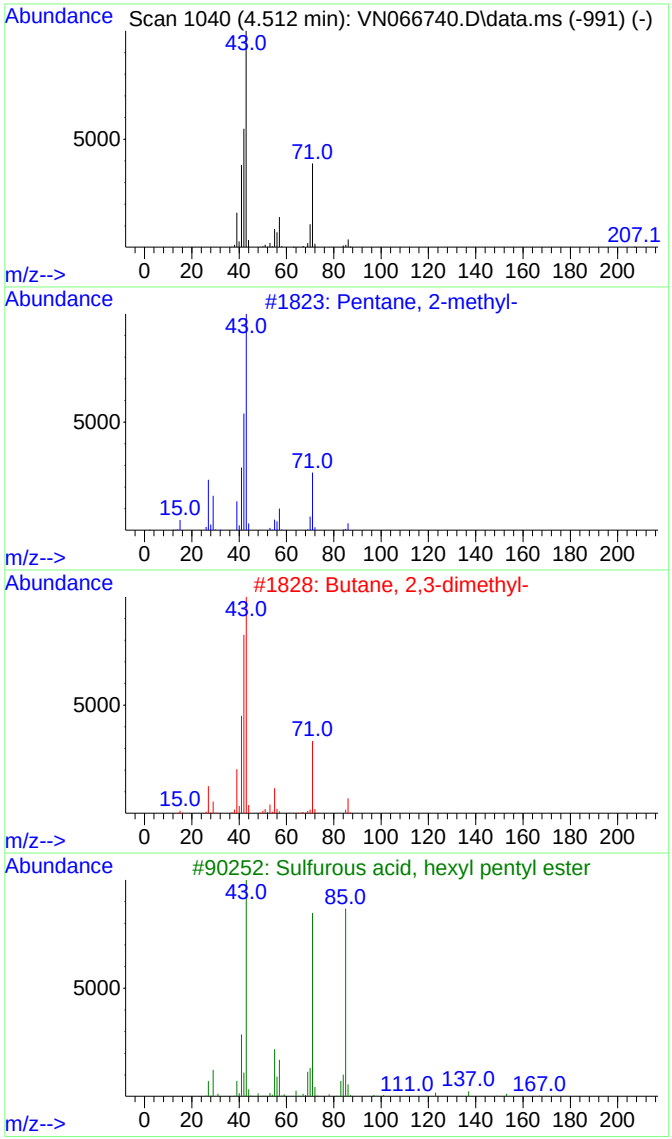
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

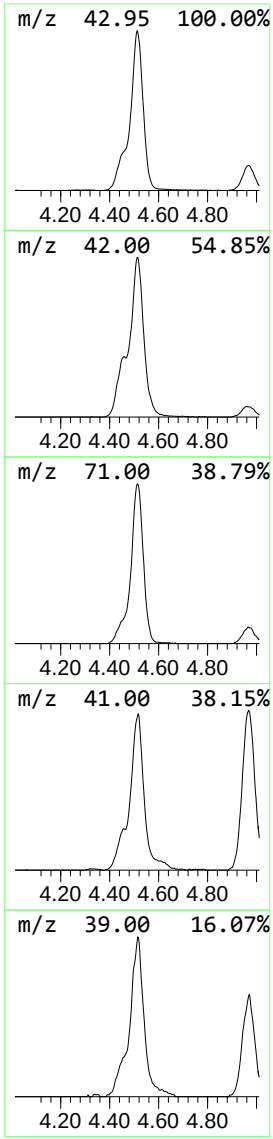
****

Peak Number 1 Pentane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.512	29.64 ug/l	1188620	Pentafluorobenzene	7.591

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	42
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	40
5	trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

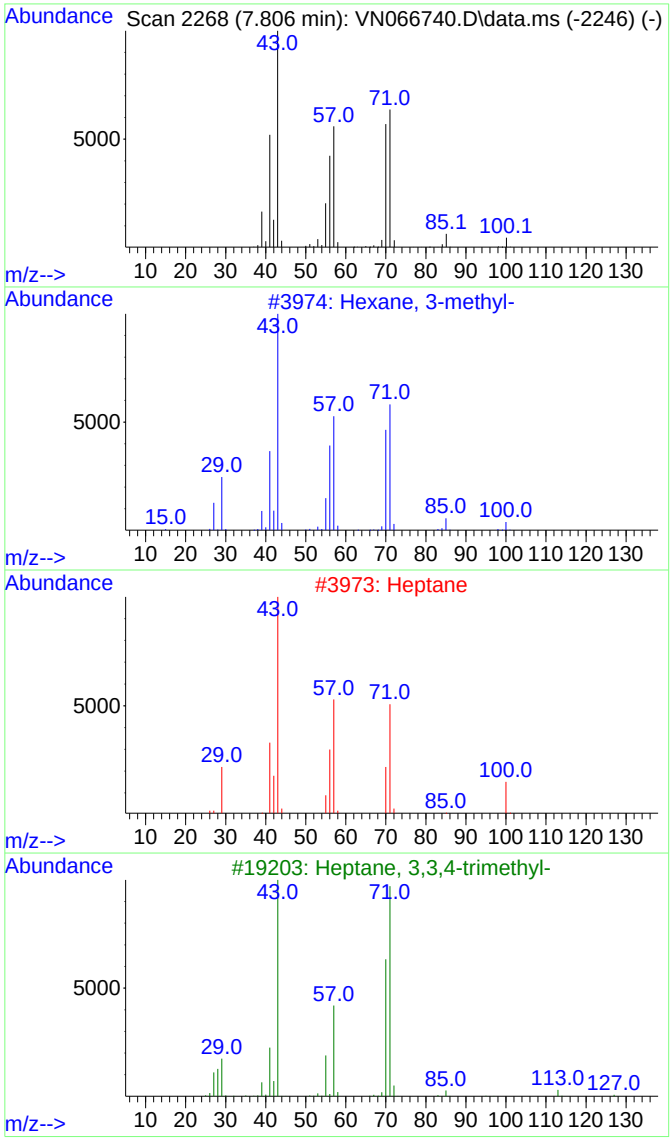
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

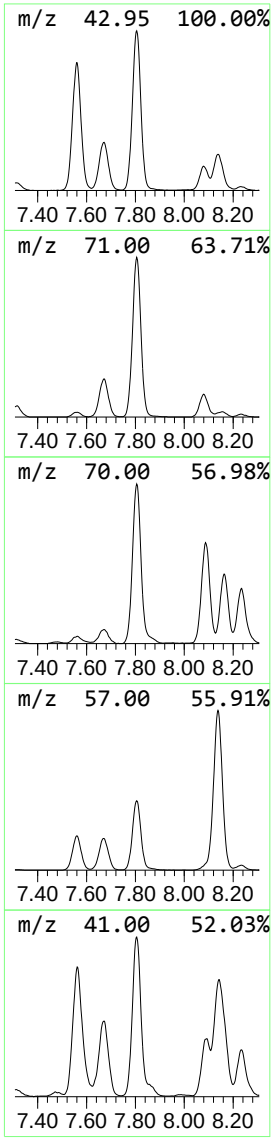
****

Peak Number 2 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.806	37.33 ug/l	1496670	Pentafluorobenzene	7.591

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	94
2	Heptane	100	C7H16	000142-82-5	80
3	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	53
4	Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

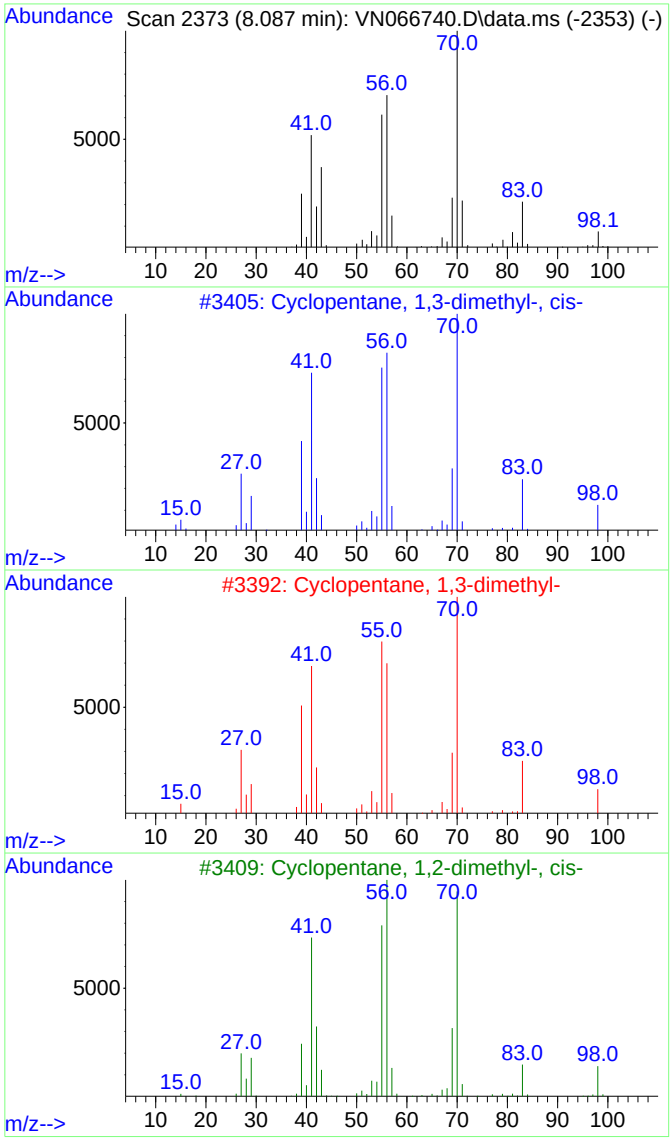
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

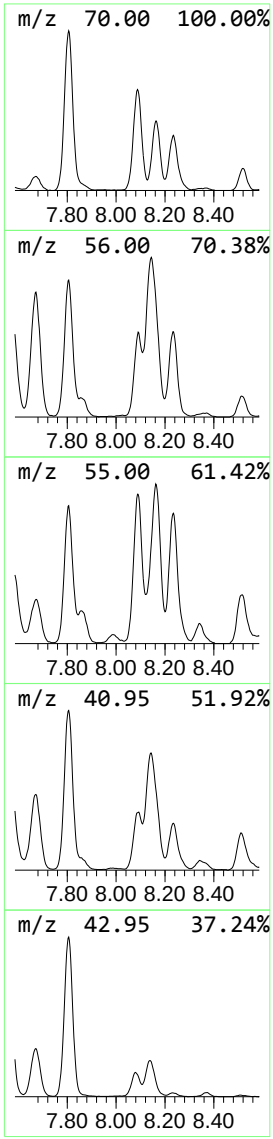
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane, 1,3-dimethyl-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.087	18.77 ug/l	562217	1,4-Difluorobenzene	8.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	92
2	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	80
3	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	60
4	Isopropylcyclobutane	98	C7H14	000872-56-0	53
5	Octane, 3-methyl-6-methylene-	140	C10H20	074630-07-2	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

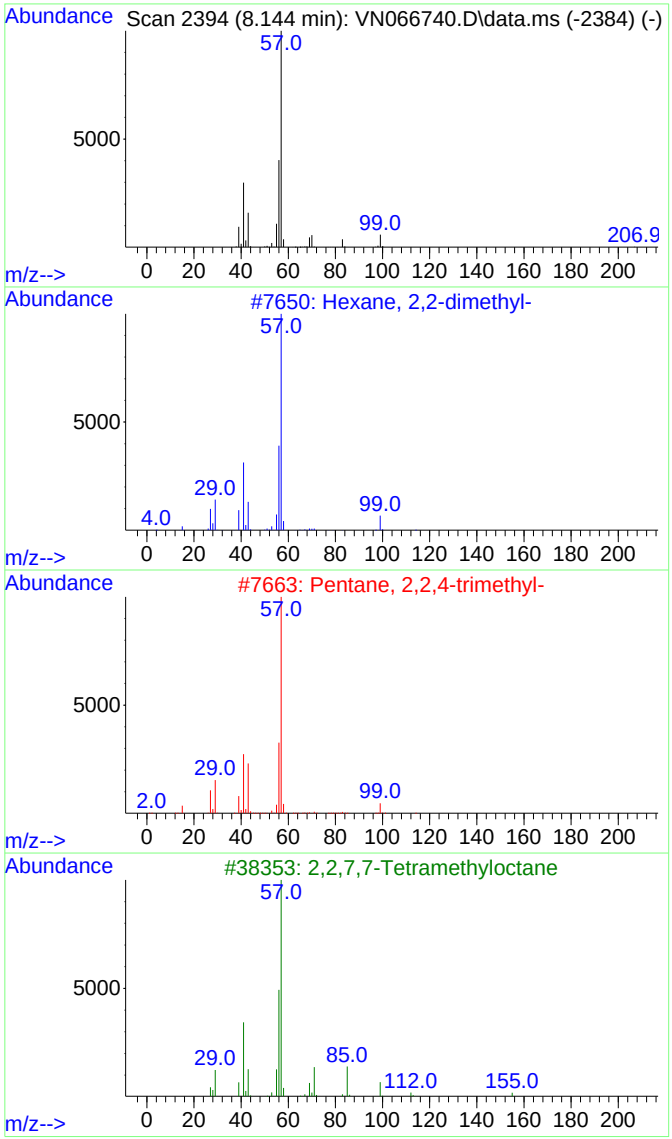
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

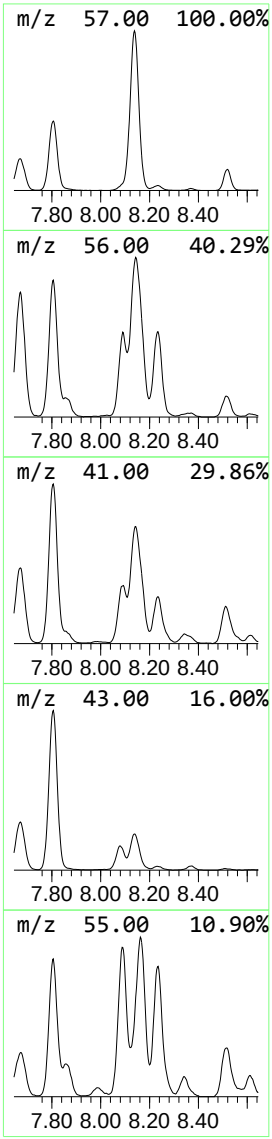
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.144	40.50 ug/l	1212980	1,4-Difluorobenzene	8.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
2	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	53
3	2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	50
4	Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50
5	Heptane, 2,2,3,5-tetramethyl-	156	C11H24	061868-42-6	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

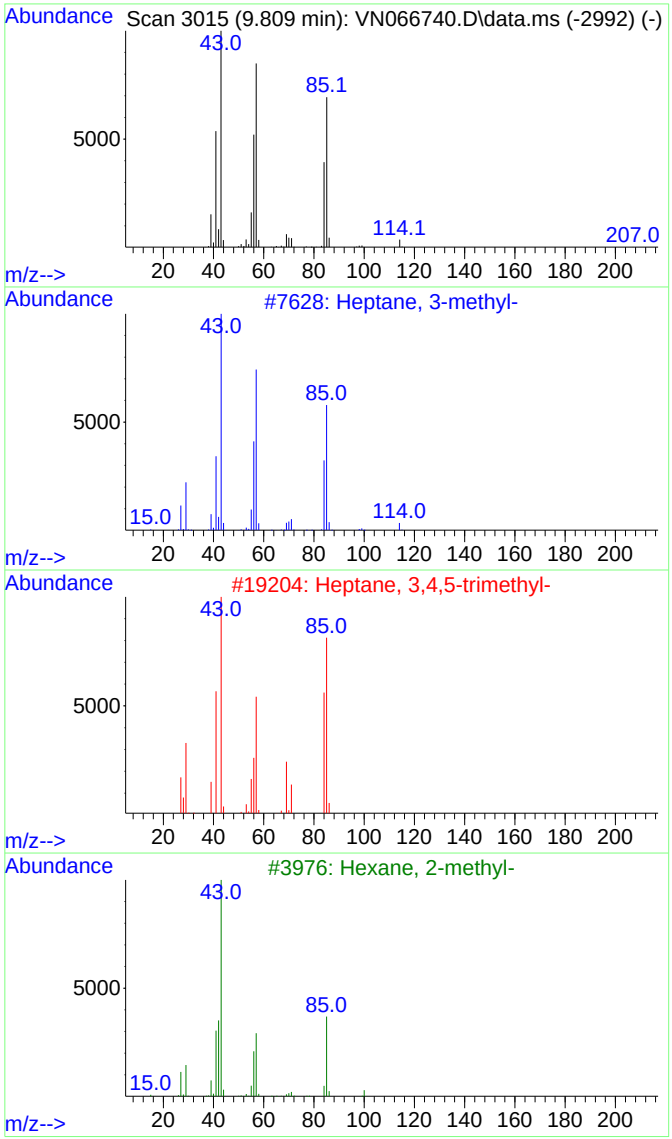
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

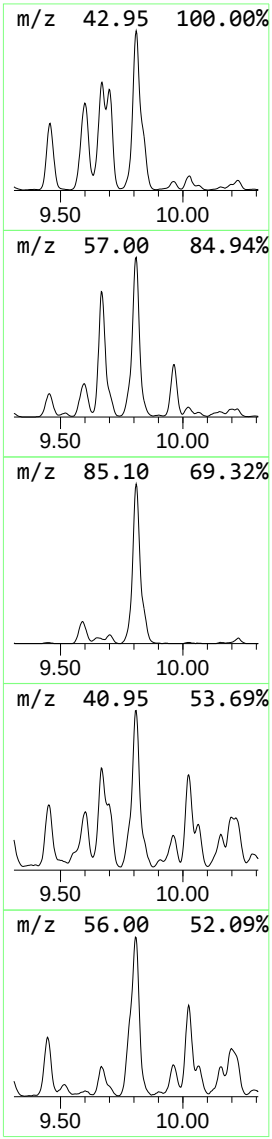
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Heptane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.809	41.70 ug/l	1248750	1,4-Difluorobenzene	8.519

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-methyl-	114	C8H18	000589-81-1	90
2	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	64
3	Hexane, 2-methyl-	100	C7H16	000591-76-4	59
4	Hexane, 2,3,3-trimethyl-	128	C9H20	016747-28-7	53
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	52





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

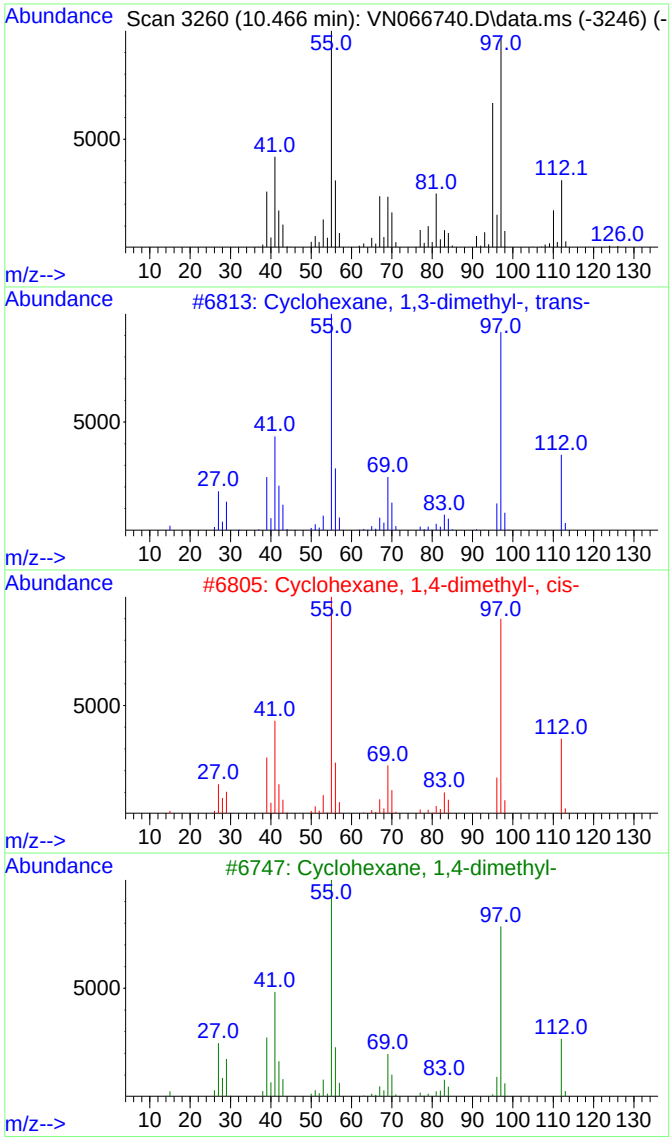
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

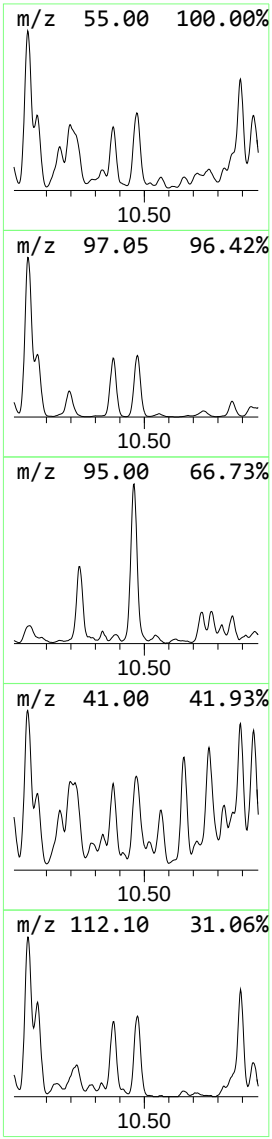
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, 1,3-dimethyl-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.466	23.23 ug/l	638701	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	93
2	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	70
3	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	70
4	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	70
5	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

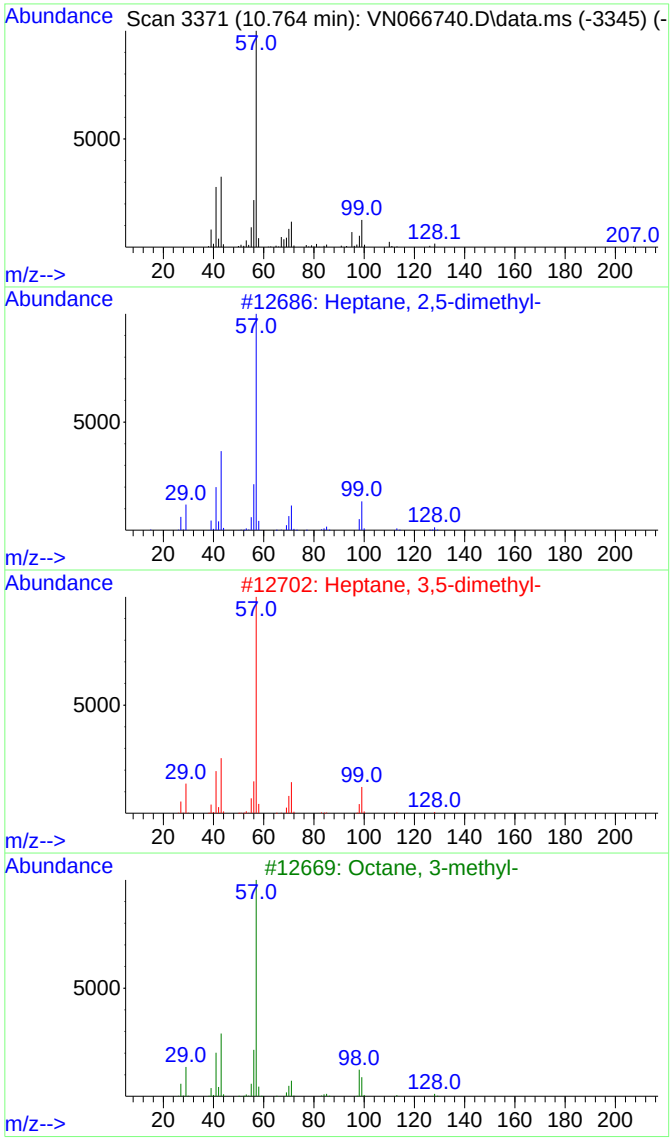
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

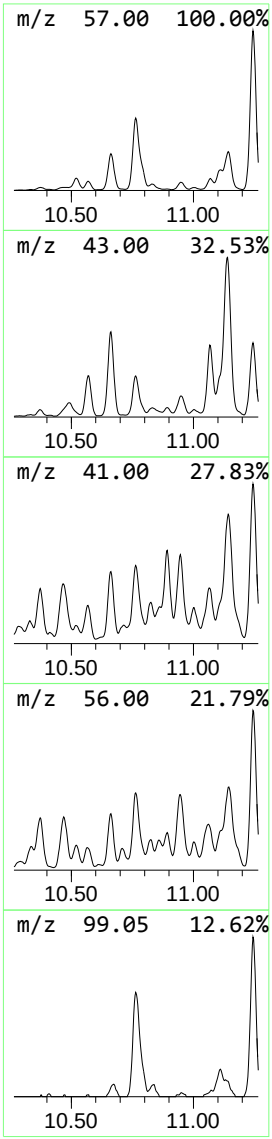
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptane, 2,5-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.764	20.26 ug/l	557288	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	87
2	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	70
3	Octane, 3-methyl-	128	C9H20	002216-33-3	68
4	Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	50
5	Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	47





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Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

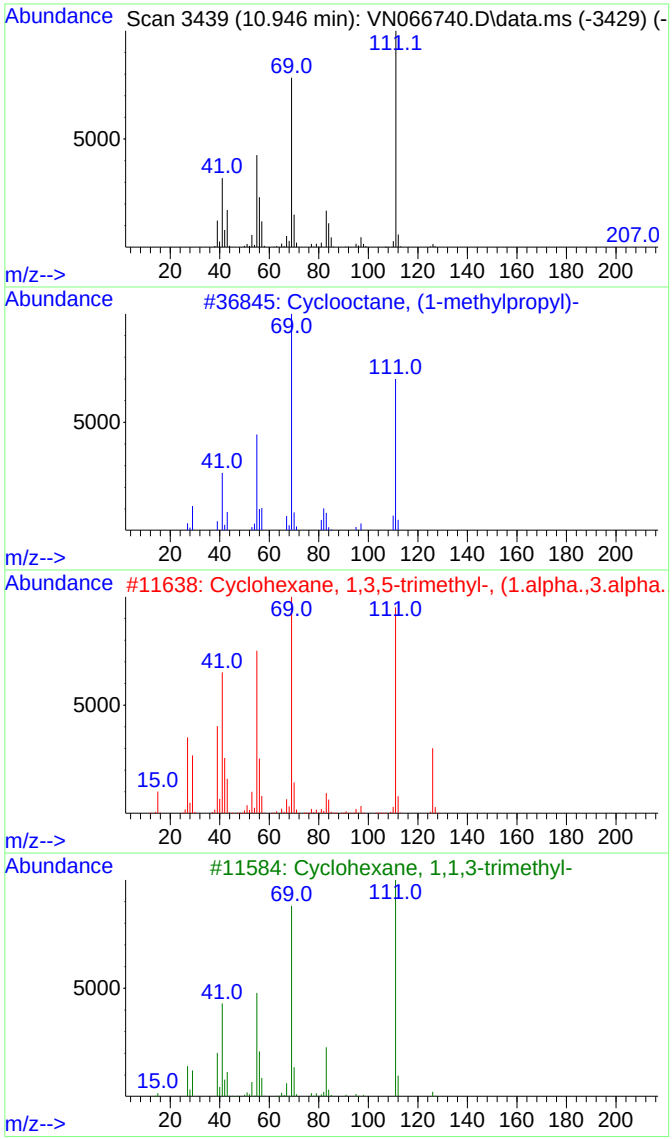
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

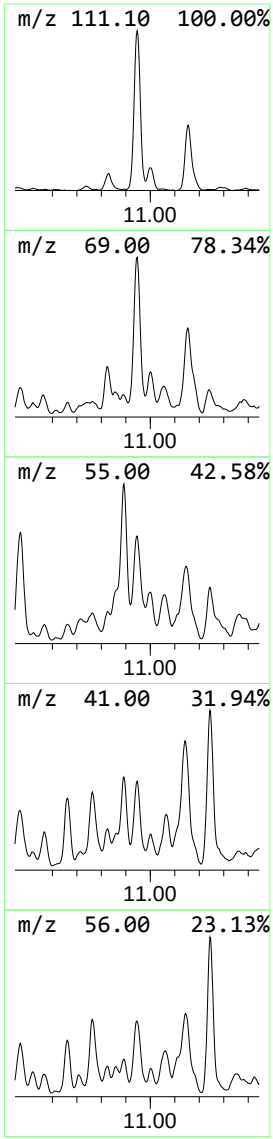
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclooctane, (1-methylpropyl)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.946	19.09 ug/l	524981	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	72
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-26-2	64
3	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	58
4	Cyclohexane, 1,2,4-trimethyl-	126	C9H18	002234-75-5	53
5	Cyclohexane, 1,2,4-trimethyl-, (...	126	C9H18	007667-60-9	53





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Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

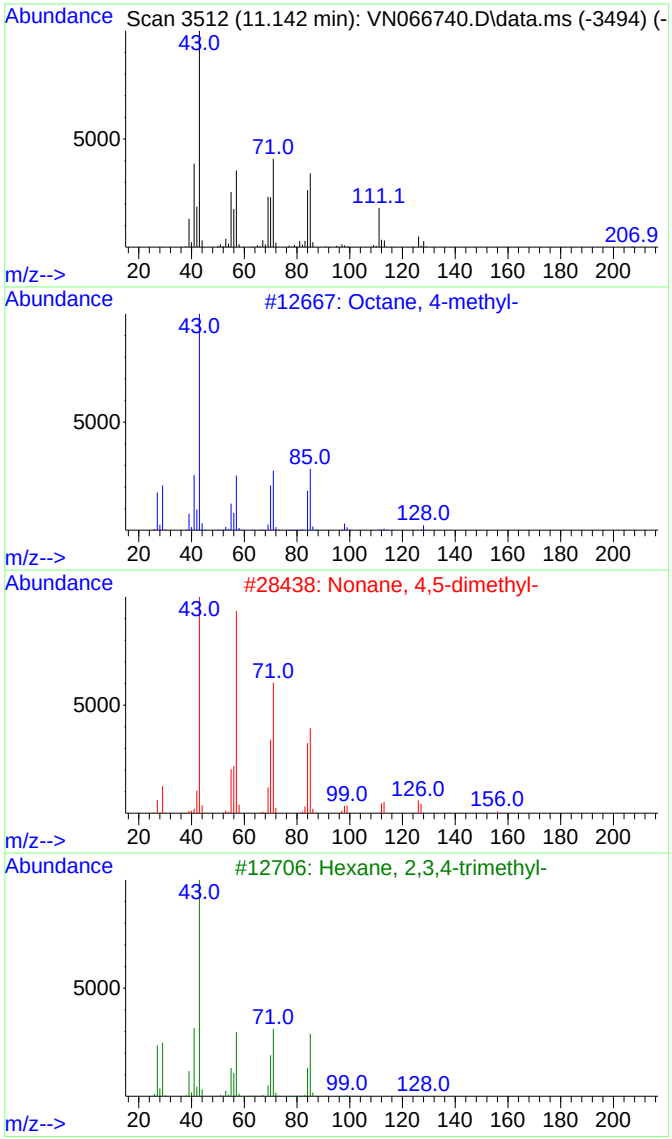
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

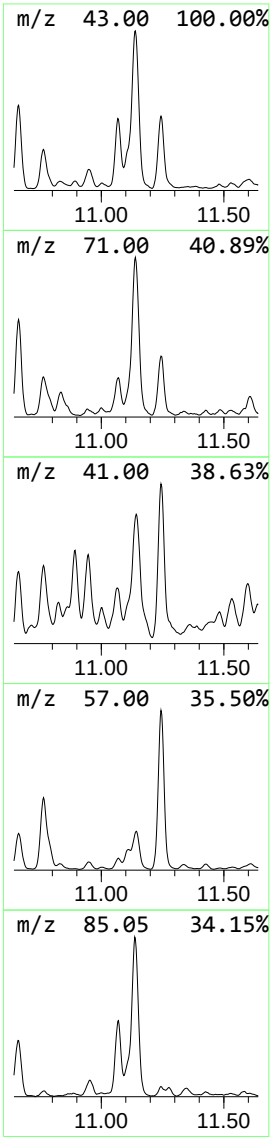
****

Peak Number 9 Octane, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.142	48.23 ug/l	1326330	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-	128	C9H20	002216-34-4	83
2	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	72
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
5	Hexane, 3-ethyl-	114	C8H18	000619-99-8	53





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Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

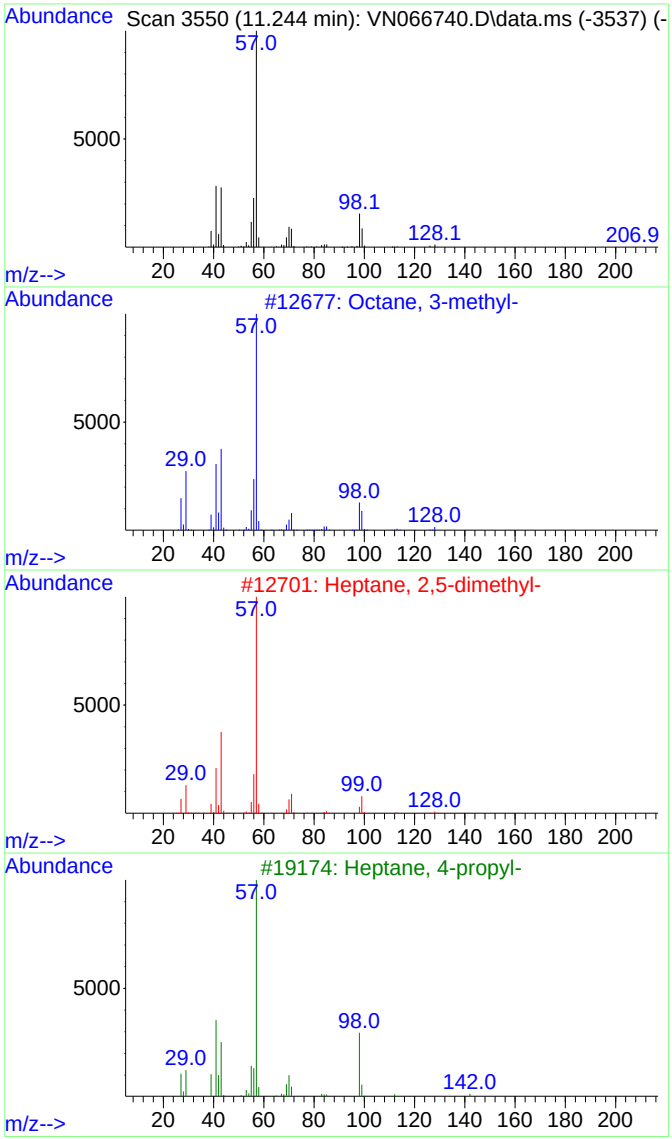
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

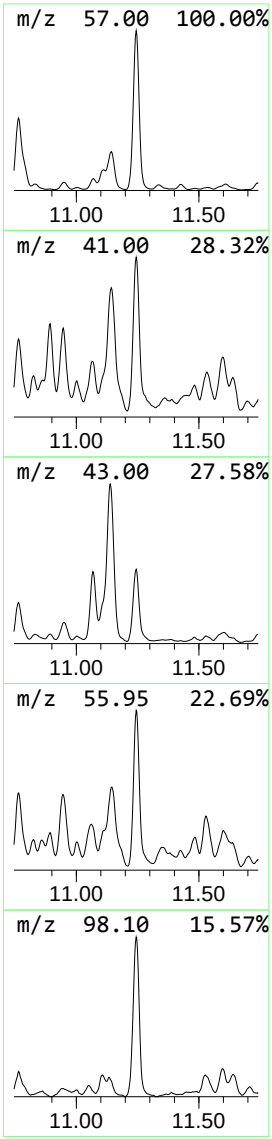
****

Peak Number 10 Octane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.244	35.02 ug/l	963188	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3-methyl-	128	C9H20	002216-33-3	90
2	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	72
3	Heptane, 4-propyl-	142	C10H22	003178-29-8	59
4	Heptane, 4-(1-methylethyl)-	142	C10H22	052896-87-4	59
5	Decane, 2,6,6-trimethyl-	184	C13H28	062108-24-1	59





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Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

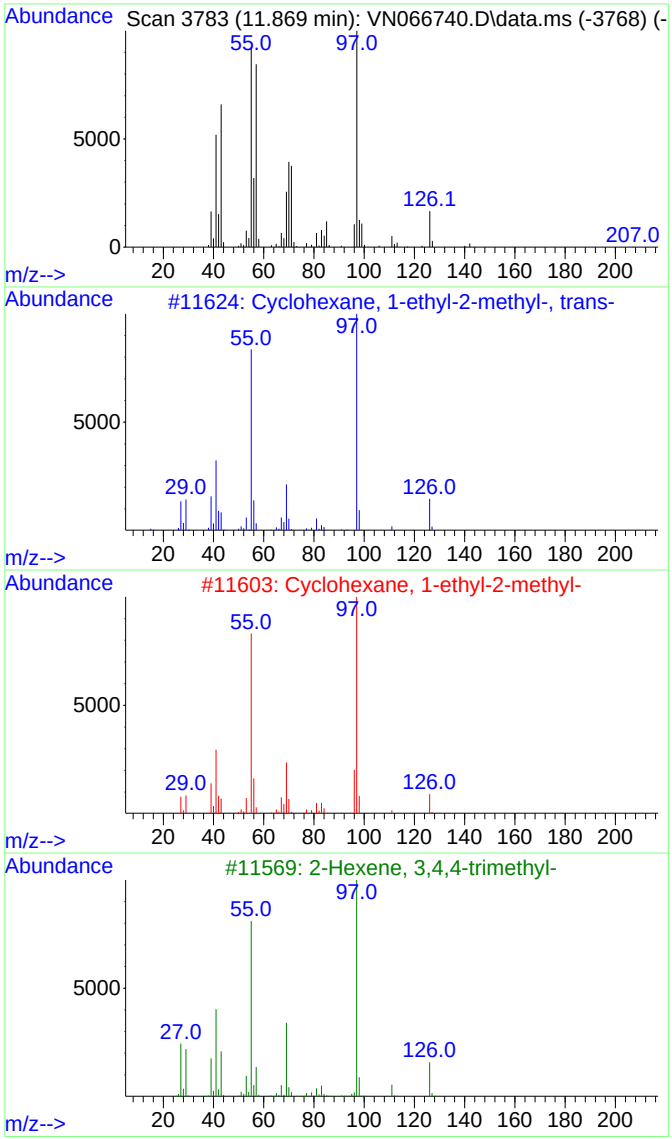
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

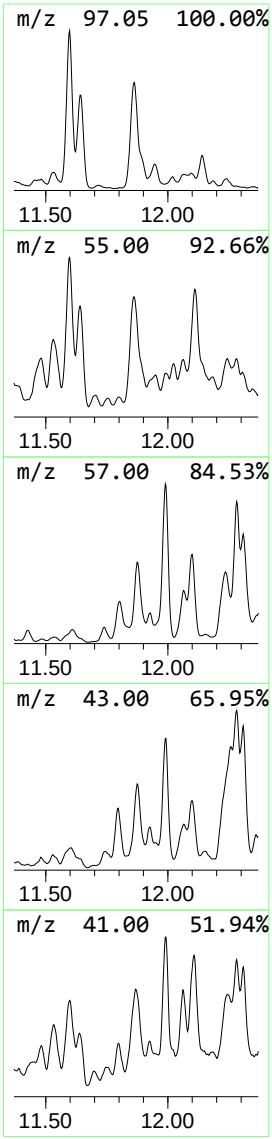
****

Peak Number 11 unknown11.869 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.869	20.96 ug/l	576511	Chlorobenzene-d5	11.349

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	45
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	45
3	2-Hexene, 3,4,4-trimethyl-	126	C9H18	053941-19-8	43
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	43
5	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

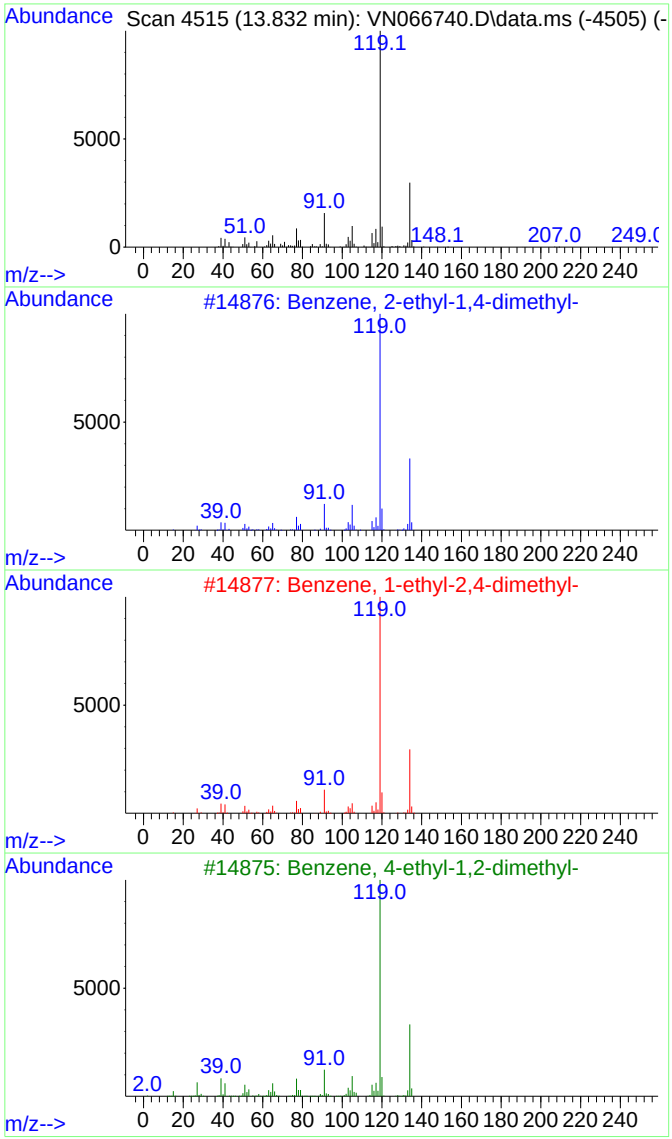
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

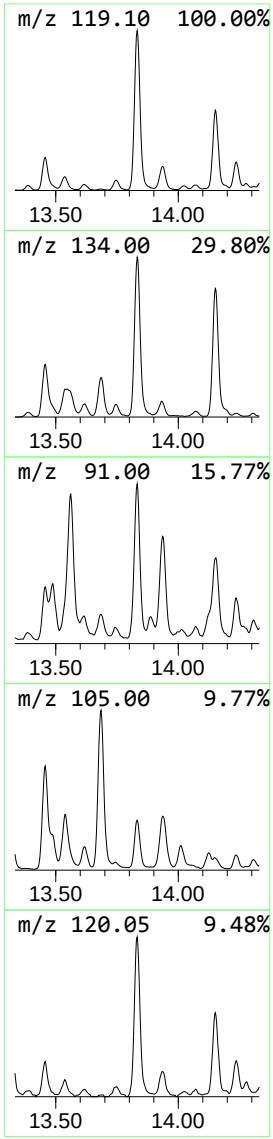
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.832	28.36 ug/l	788119	1,4-Dichlorobenzene-d4	13.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	97
2	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
3	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	95
4	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
5	o-Cymene	134	C10H14	000527-84-4	95





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Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

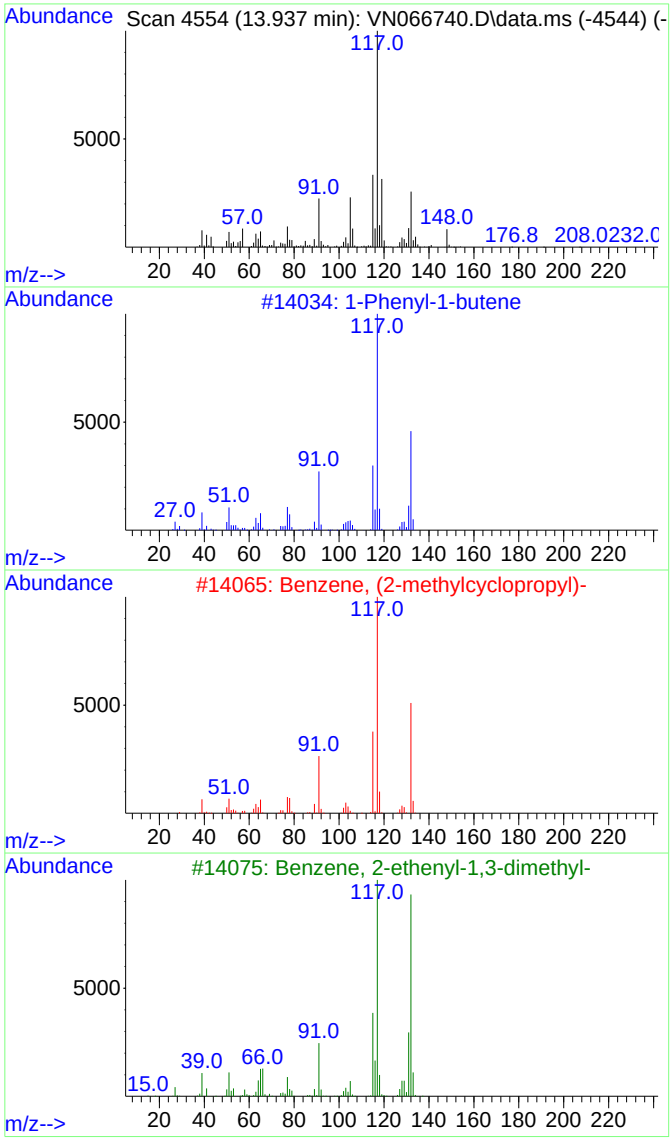
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

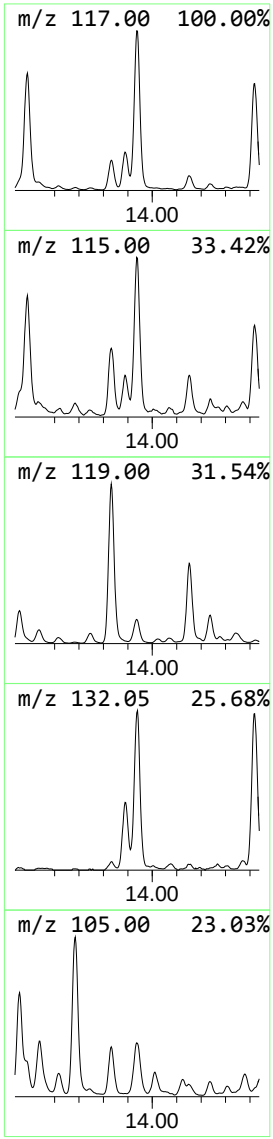
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 1-Phenyl-1-butene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.937	21.47 ug/l	596710	1,4-Dichlorobenzene-d4	13.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-butene	132	C10H12	000824-90-8	70
2	Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	70
3	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	70
4	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	68
5	Indan, 1-methyl-	132	C10H12	000767-58-8	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

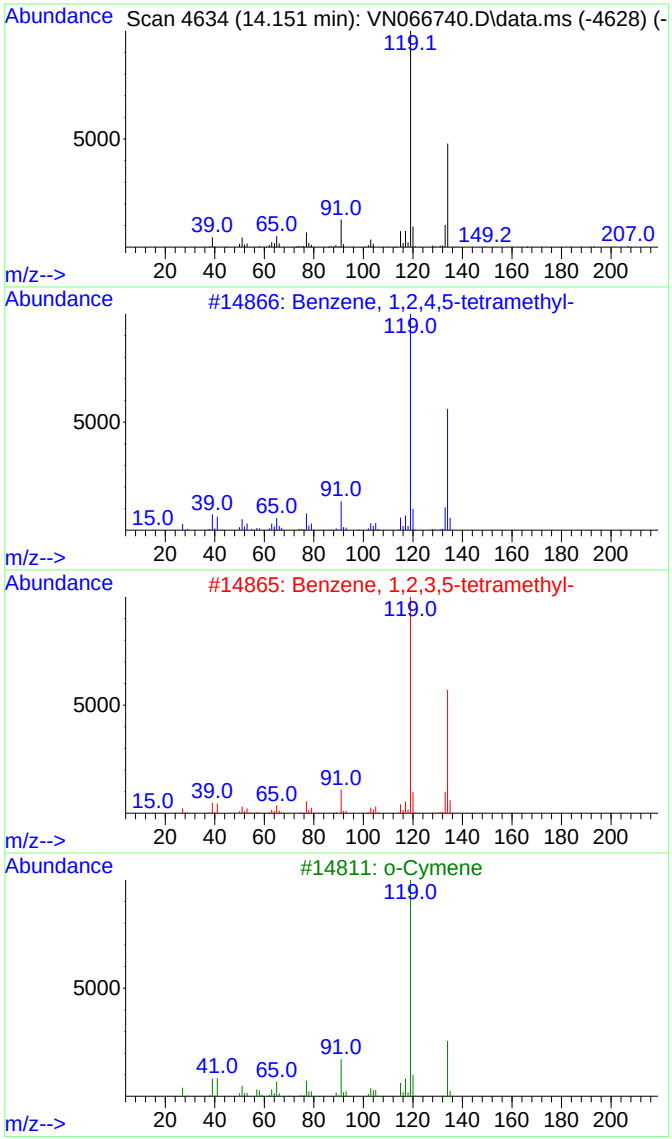
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

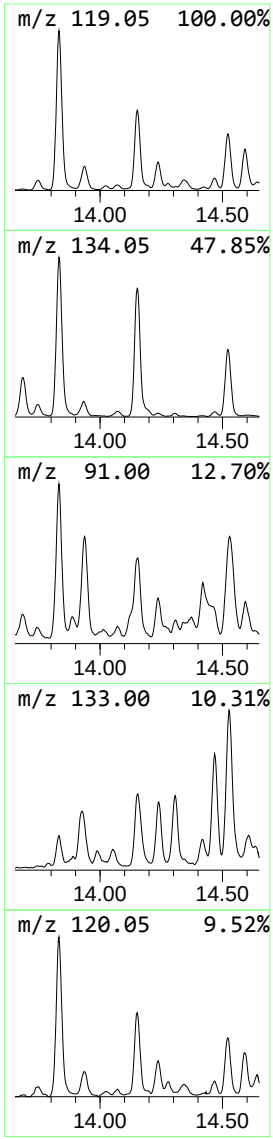
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	20.39 ug/l	566721	1,4-Dichlorobenzene-d4	13.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	o-Cymene	134	C10H14	000527-84-4	94
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
124-SB-1

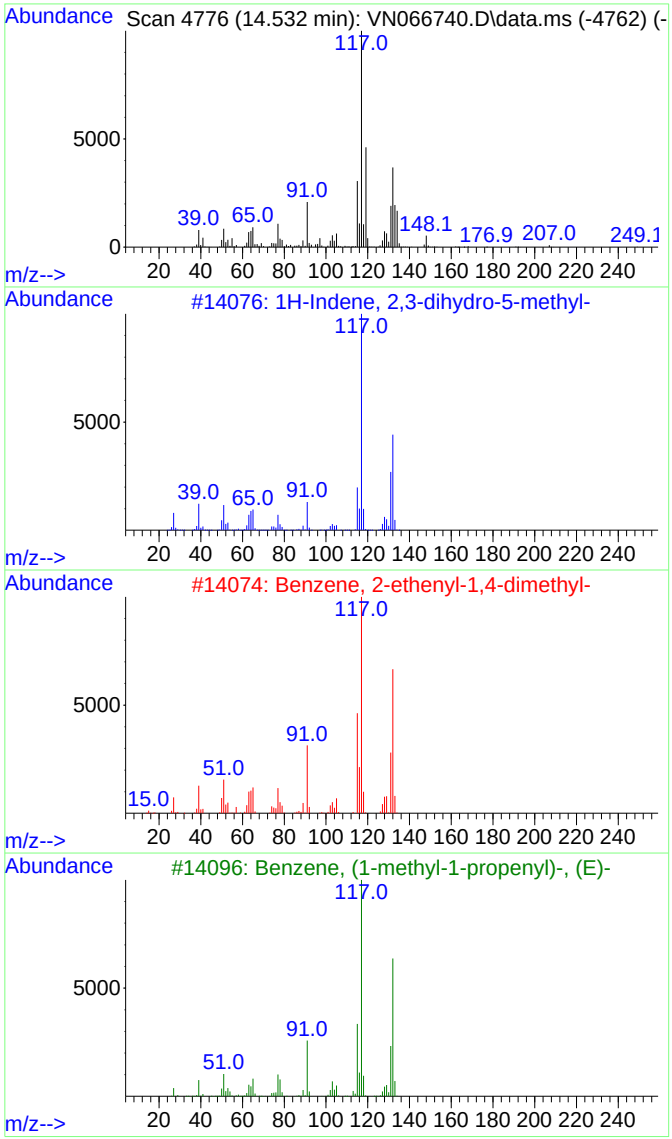
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.M
Quant Title : SW846 8260

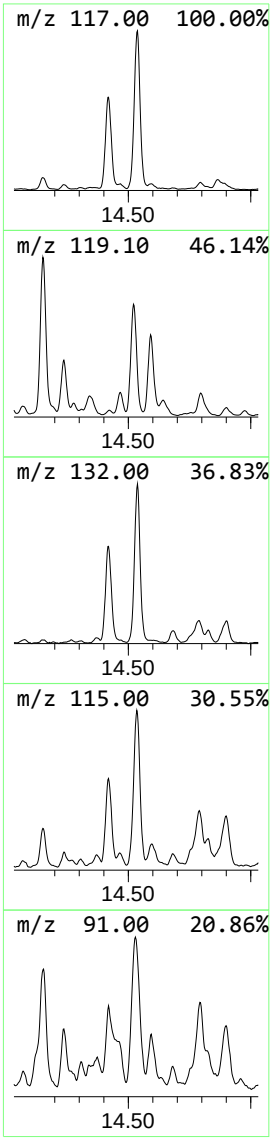
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.532	34.49 ug/l	958606	1,4-Dichlorobenzene-d4	13.288

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	91
2	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	86
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042321\
Data File : VN066740.D
Acq On : 23 Apr 2021 16:13
Operator : JC/MD
Sample : M2047-06 10X
Misc : 6.97g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 124-SB-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042121W.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
Pentane, 2-methyl-	4.512	29.6	ug/l	1188620	1	7.591	2004840	50.0
Hexane, 3-methyl-	7.806	37.3	ug/l	1496670	1	7.591	2004840	50.0
Cyclopentane, 1...	8.087	18.8	ug/l	562217	2	8.519	1497380	50.0
Hexane, 2,2-dim...	8.144	40.5	ug/l	1212980	2	8.519	1497380	50.0
Heptane, 3-methyl-	9.809	41.7	ug/l	1248750	2	8.519	1497380	50.0
Cyclohexane, 1,...	10.466	23.2	ug/l	638701	3	11.349	1375020	50.0
Heptane, 2,5-di...	10.764	20.3	ug/l	557288	3	11.349	1375020	50.0
Cyclooctane, (1...	10.946	19.1	ug/l	524981	3	11.349	1375020	50.0
Octane, 4-methyl-	11.142	48.2	ug/l	1326330	3	11.349	1375020	50.0
Octane, 3-methyl-	11.244	35.0	ug/l	963188	3	11.349	1375020	50.0
unknown11.869	11.869	21.0	ug/l	576511	3	11.349	1375020	50.0
Benzene, 2-ethy...	13.832	28.4	ug/l	788119	4	13.288	1389730	50.0
1-Phenyl-1-butene	13.937	21.5	ug/l	596710	4	13.288	1389730	50.0
Benzene, 1,2,4,...	14.151	20.4	ug/l	566721	4	13.288	1389730	50.0
1H-Indene, 2,3-...	14.532	34.5	ug/l	958606	4	13.288	1389730	50.0