

Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
 Data File : VN052858.D
 Acq On : 13 Dec 2018 12:27
 Operator : MD\SY
 Sample : J6319-02
 Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 28

Instrument :
 MSVOA_N
 ClientSampleId :
 056_BT-1-2

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.584	834	874	927	rVB	627971	2739224	5.18%	0.388%
2	5.050	989	1019	1059	rBV	558950	1998453	3.78%	0.283%
3	6.365	1402	1428	1446	rBV8	189085	685730	1.30%	0.097%
4	6.516	1458	1475	1490	rBV2	260944	785646	1.49%	0.111%
5	6.625	1491	1509	1527	rBV	1049353	3157330	5.97%	0.447%
6	7.323	1708	1726	1736	rVV	276022	746137	1.41%	0.106%
7	7.387	1738	1746	1768	rVB4	217568	576737	1.09%	0.082%
8	7.638	1773	1824	1844	rBV8	4666327	17921582	33.88%	2.539%
9	7.741	1844	1856	1878	rVB2	1556295	4230800	8.00%	0.599%
10	7.873	1878	1897	1911	rBV	4796346	11846903	22.40%	1.679%
11	8.027	1931	1945	1966	rVB2	719649	1839574	3.48%	0.261%
12	8.156	1967	1985	1997	rBV2	2760823	6814099	12.88%	0.966%
13	8.233	1997	2009	2019	rVV4	2488389	5969643	11.29%	0.846%
14	8.301	2020	2030	2051	rVB	3010811	7195866	13.60%	1.020%
15	8.410	2052	2064	2095	rVB4	352525	1183009	2.24%	0.168%
16	8.580	2097	2117	2141	rBV3	3573254	9933487	18.78%	1.408%
17	8.744	2158	2168	2178	rVB2	413286	763536	1.44%	0.108%
18	8.818	2178	2191	2201	rBV	2079652	4528292	8.56%	0.642%
19	9.079	2246	2272	2285	rBV2	21281182	52895504	100.00%	7.495%
20	9.143	2285	2292	2307	rVB2	2103721	4090819	7.73%	0.580%
21	9.272	2308	2332	2345	rBV3	3483018	8583263	16.23%	1.216%
22	9.365	2346	2361	2375	rVB2	3420479	7926080	14.98%	1.123%
23	9.436	2376	2383	2395	rBV7	468169	1006614	1.90%	0.143%
24	9.509	2396	2406	2419	rVB3	4133067	8043180	15.21%	1.140%
25	9.616	2420	2439	2446	rBV3	2198867	4680504	8.85%	0.663%
26	9.664	2446	2454	2463	rBV2	2973003	4801343	9.08%	0.680%
27	9.728	2463	2474	2498	rVB2	13686356	35583684	67.27%	5.042%
28	9.870	2498	2518	2540	rBV	8878598	23365587	44.17%	3.311%
29	9.969	2540	2549	2555	rBV2	1448911	2668540	5.04%	0.378%
30	10.024	2556	2566	2575	rVB2	5259330	8942477	16.91%	1.267%
31	10.088	2575	2586	2594	rBV2	15112234	29170843	55.15%	4.133%
32	10.214	2610	2625	2631	rBV2	2761989	5541937	10.48%	0.785%
33	10.259	2631	2639	2641	rBV3	3551291	4628010	8.75%	0.656%
34	10.349	2660	2667	2670	rBV3	664249	915589	1.73%	0.130%

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35	10.387	2672	2679	2685	rVV4	2743611	4532067	8.57%	0.642%
36	10.432	2685	2693	2709	rVB	6540942	11763581	22.24%	1.667%
37	10.526	2710	2722	2735	rBV4	6903414	15751529	29.78%	2.232%
38	10.625	2745	2753	2763	rVB4	2625260	4588103	8.67%	0.650%
39	10.718	2763	2782	2792	rBV	6880898	12803743	24.21%	1.814%
40	10.825	2793	2815	2825	rVV2	4808203	13413413	25.36%	1.901%
41	10.882	2826	2833	2838	rVV6	3378060	5850971	11.06%	0.829%
42	10.918	2840	2844	2847	rVV2	3453116	4343872	8.21%	0.615%
43	10.953	2848	2855	2863	rVV	10393600	18020983	34.07%	2.553%
44	11.005	2863	2871	2882	rVV	11003648	20450398	38.66%	2.898%
45	11.062	2882	2889	2897	rVV4	2924625	5198180	9.83%	0.737%
46	11.120	2897	2907	2916	rVV5	4820102	9434309	17.84%	1.337%
47	11.201	2916	2932	2952	rVB5	13736420	34020301	64.32%	4.820%
48	11.300	2952	2963	2987	rBV	10623513	20978413	39.66%	2.972%
49	11.410	2988	2997	3006	rBV3	3448356	6198639	11.72%	0.878%
50	11.593	3045	3054	3063	rVB6	3463505	6792786	12.84%	0.962%
51	11.654	3064	3073	3081	rBV	6174463	11154139	21.09%	1.580%
52	11.754	3096	3104	3112	rBV6	1271282	2295472	4.34%	0.325%
53	11.812	3114	3122	3128	rBV5	1460816	2466926	4.66%	0.350%
54	11.857	3130	3136	3144	rVB5	1275627	1899597	3.59%	0.269%
55	11.921	3144	3156	3169	rBV6	5718976	13845287	26.17%	1.962%
56	12.046	3188	3195	3202	rVB	5650805	7567877	14.31%	1.072%
57	12.120	3210	3218	3224	rBV4	4489639	7249418	13.71%	1.027%
58	12.162	3224	3231	3241	rVB4	6451568	11131537	21.04%	1.577%
59	12.403	3301	3306	3312	rVB3	1835072	2284186	4.32%	0.324%
60	12.445	3313	3319	3327	rVB	3888245	4930396	9.32%	0.699%
61	12.564	3348	3356	3359	rBV3	3277645	4672109	8.83%	0.662%
62	12.725	3394	3406	3416	rBV6	4675040	11085585	20.96%	1.571%
63	12.924	3462	3468	3473	rBV4	2210285	3287558	6.22%	0.466%
64	12.963	3474	3480	3494	rVB3	6466281	10207483	19.30%	1.446%
65	13.149	3532	3538	3541	rBV3	1680577	2273104	4.30%	0.322%
66	13.426	3618	3624	3634	rVB3	2495700	3751767	7.09%	0.532%
67	13.513	3645	3651	3656	rBV	2998444	4052433	7.66%	0.574%
68	13.612	3670	3682	3689	rBV3	2828659	7006635	13.25%	0.993%
69	13.667	3690	3699	3708	rVV5	4422371	8125444	15.36%	1.151%
70	13.889	3760	3768	3778	rVB	11325544	16651881	31.48%	2.359%
71	13.995	3792	3801	3812	rVB	9674891	16046798	30.34%	2.274%

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Integration Parameters: RTEINT.P

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Smoothing : ON Filtering: 5
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Title : SW846 8260

72	14.294	3886	3894	3901	rBV2	3736779	5872399	11.10%	0.832%
73	14.477	3943	3951	3961	rBV2	4921098	8733052	16.51%	1.237%
74	14.593	3975	3987	3997	rBV4	10101632	20757823	39.24%	2.941%
75	14.648	3998	4004	4015	rVB2	3371381	5580520	10.55%	0.791%
76	14.850	4051	4067	4075	rBV4	5787189	11462560	21.67%	1.624%
77	14.959	4091	4101	4113	rVB2	4739909	10138023	19.17%	1.436%
78	15.242	4180	4189	4196	rBV3	1860062	3116870	5.89%	0.442%
79	15.419	4233	4244	4257	rBV2	2065014	4105067	7.76%	0.582%
80	15.763	4343	4351	4363	rVB7	843104	1813532	3.43%	0.257%
81	15.908	4388	4396	4406	rVB4	380262	682215	1.29%	0.097%
82	16.352	4523	4534	4559	rVB	664755	1600876	3.03%	0.227%

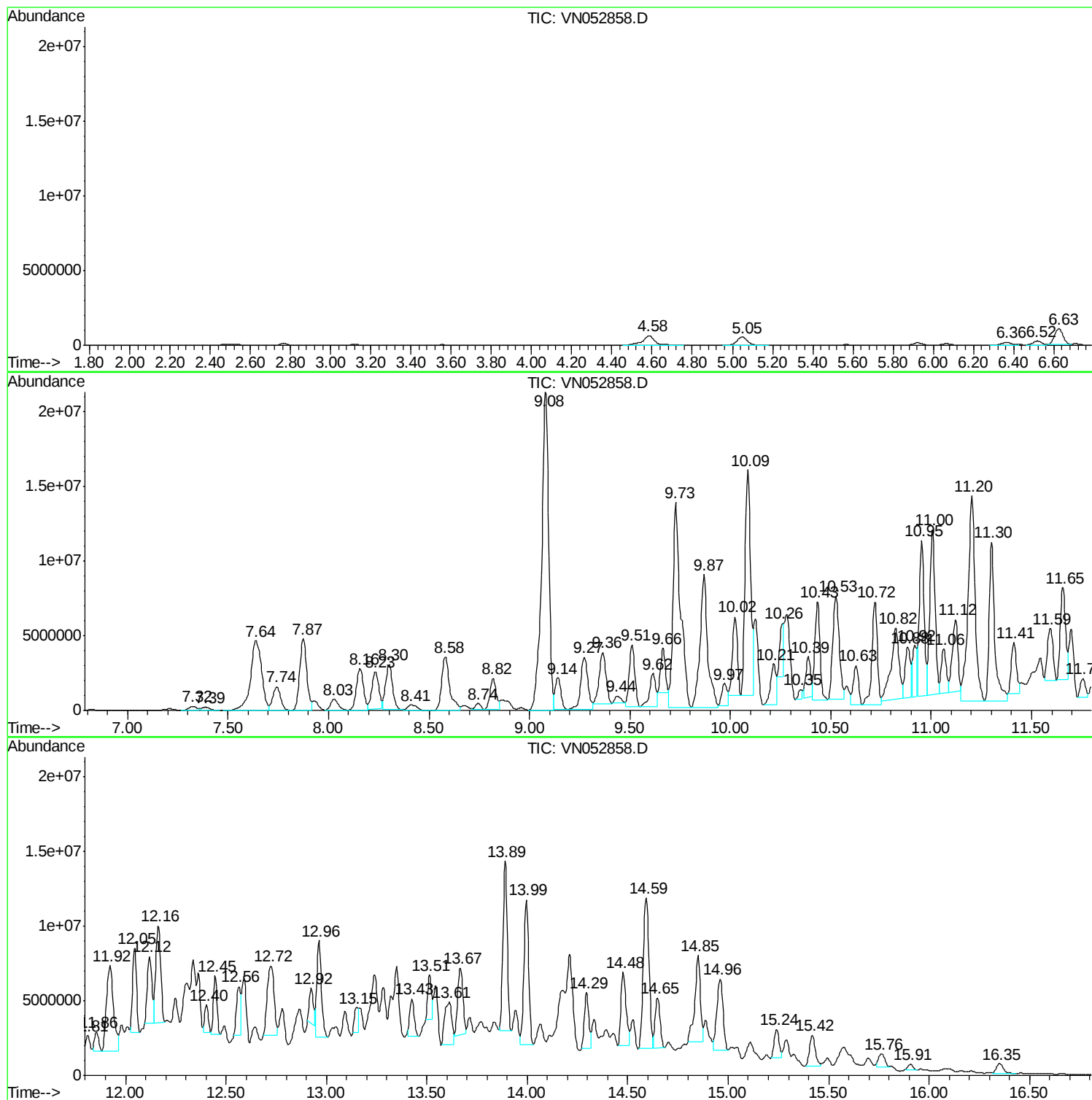
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

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



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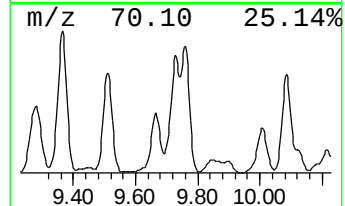
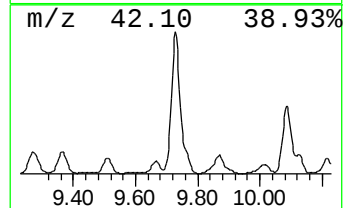
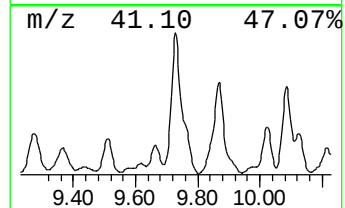
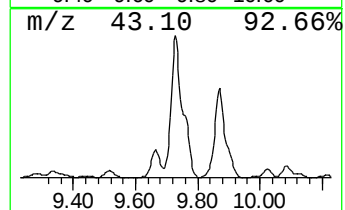
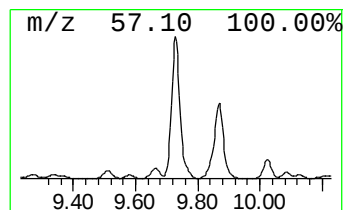
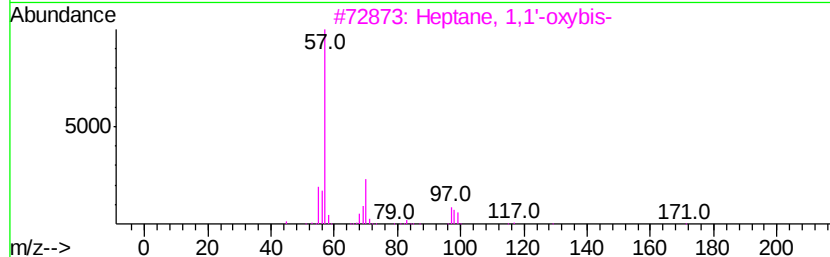
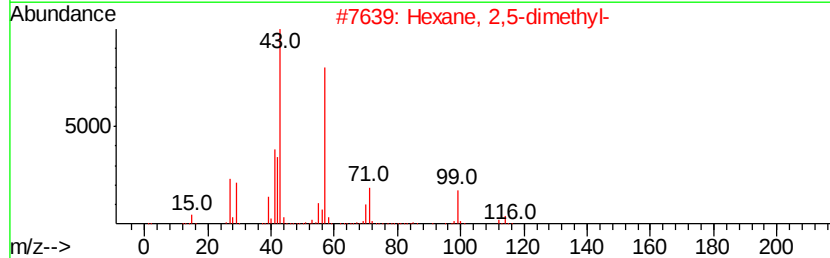
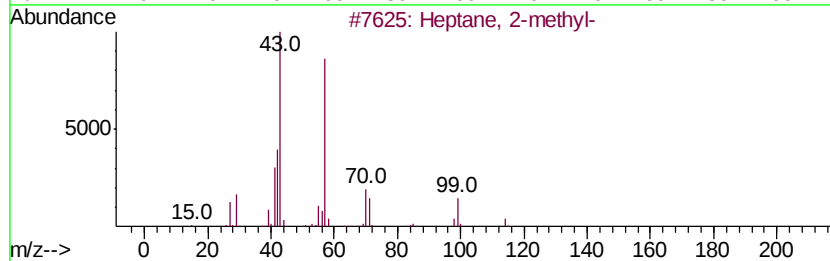
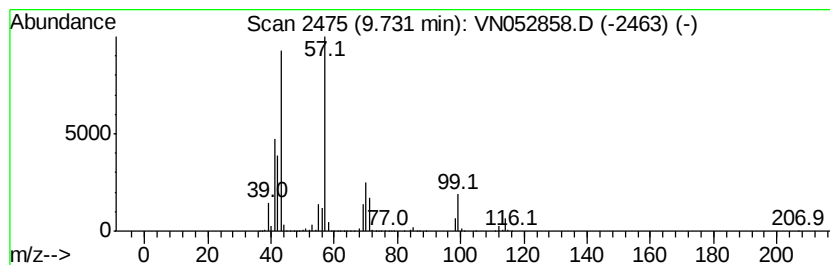
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

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

Peak Number 1 Heptane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.73	179.11 ug/l	35583700	1,4-Difluorobenzene	8.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptane, 2-methyl-	114	C8H18	000592-27-8	94
2		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	81
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4		Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	37
5		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	35



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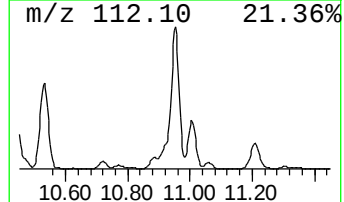
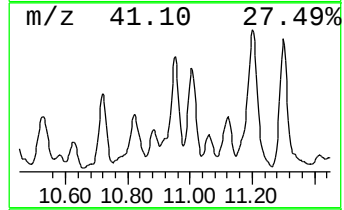
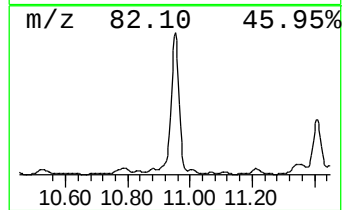
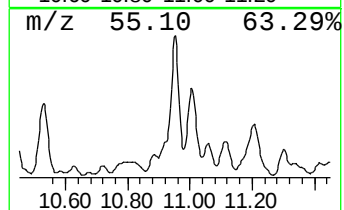
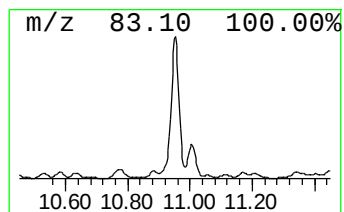
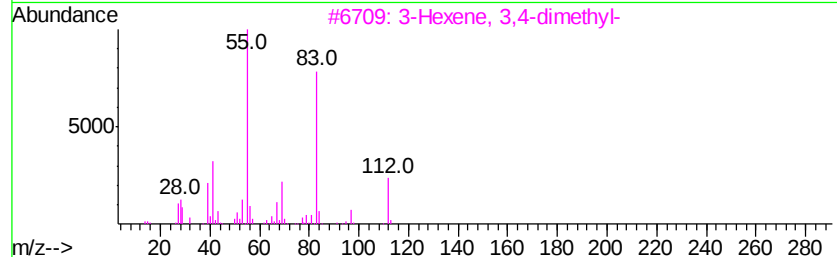
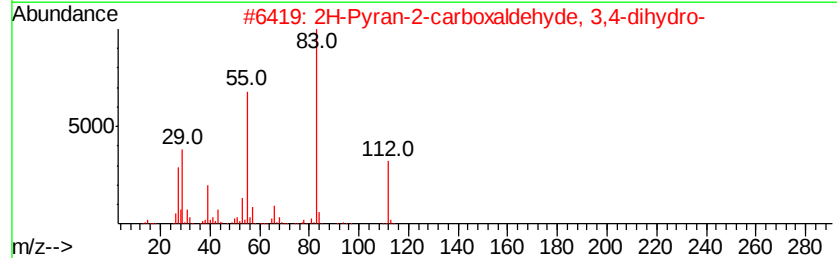
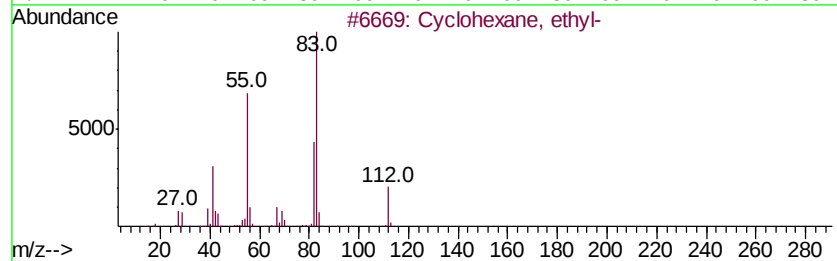
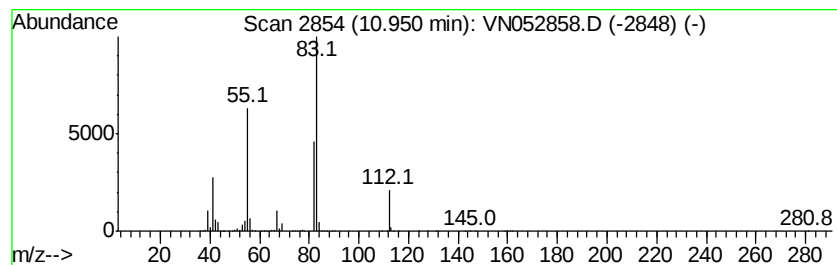
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexane, ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	145.36 ug/l	18021000	Chlorobenzene-d5	11.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexane, ethyl-	112 C8H16	001678-91-7 86
2		2H-Pyran-2-carboxaldehyde, 3,4-d...	112 C6H8O2	000100-73-2 50
3		3-Hexene, 3,4-dimethyl-	112 C8H16	030951-95-2 50
4		Cyclohexane, octyl-	196 C14H28	001795-15-9 50
5		2H-Pyran-2-carboxaldehyde, 5,6-d...	112 C6H8O2	053897-26-0 50



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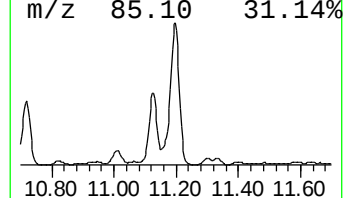
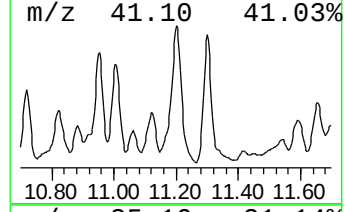
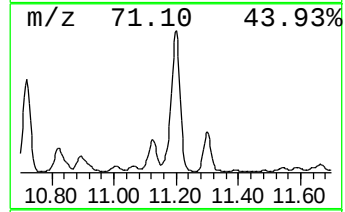
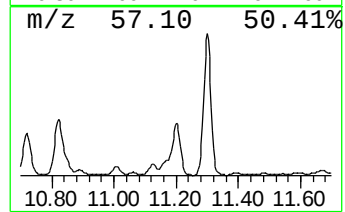
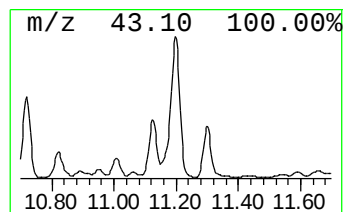
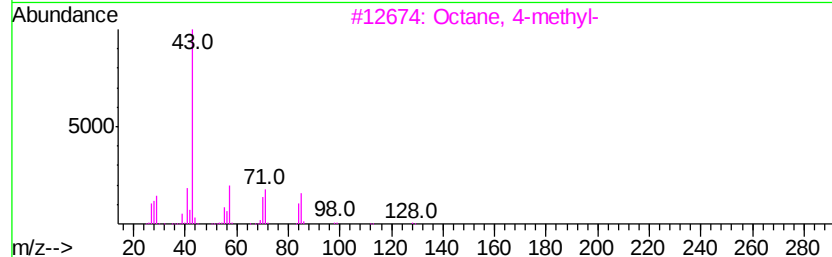
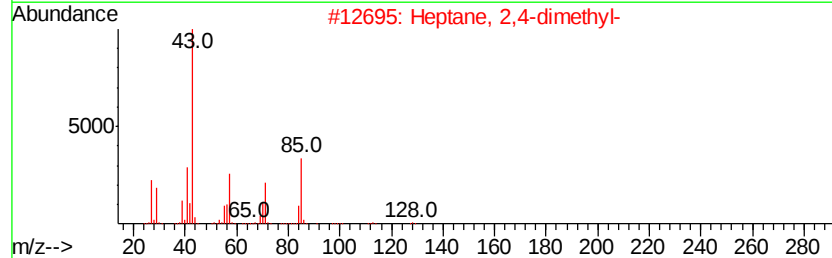
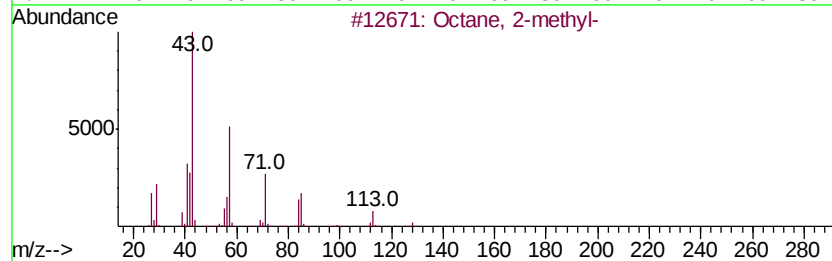
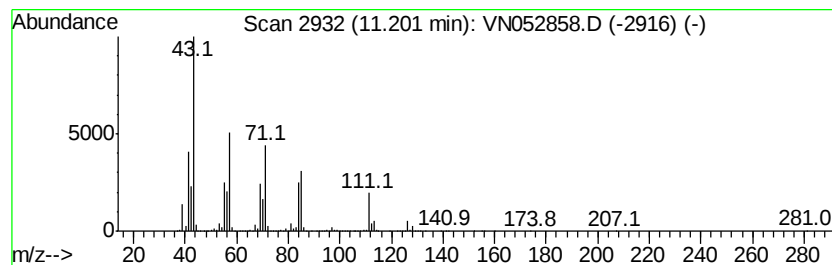
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

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

Peak Number 4 Octane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	274.42 ug/l	34020300	Chlorobenzene-d5	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octane, 2-methyl-	128	C9H20	003221-61-2	64
2		Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	49
3		Octane, 4-methyl-	128	C9H20	002216-34-4	43
4		Hexane, 2,3,5-trimethyl-	128	C9H20	001069-53-0	43
5		Octane, 3-ethyl-2,7-dimethyl-	170	C12H26	062183-55-5	43



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056_BT-1-2

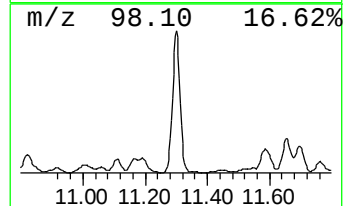
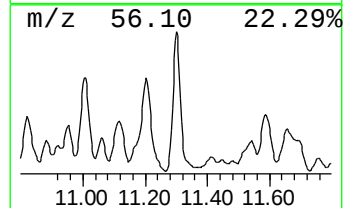
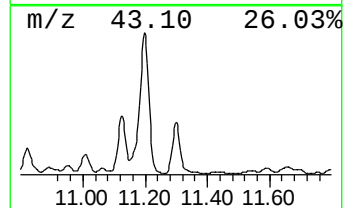
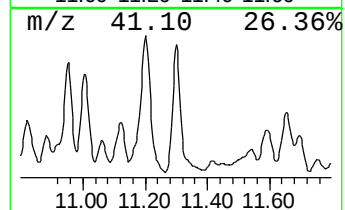
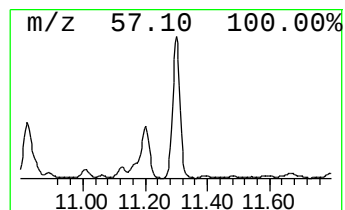
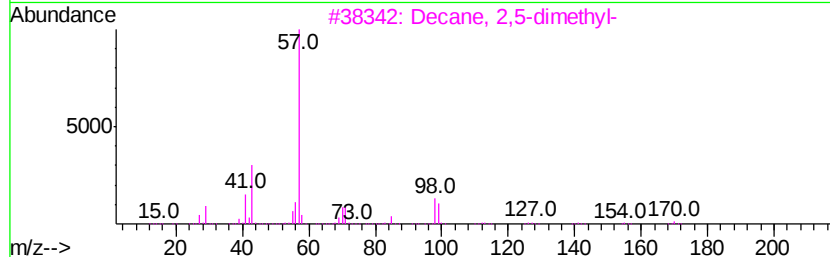
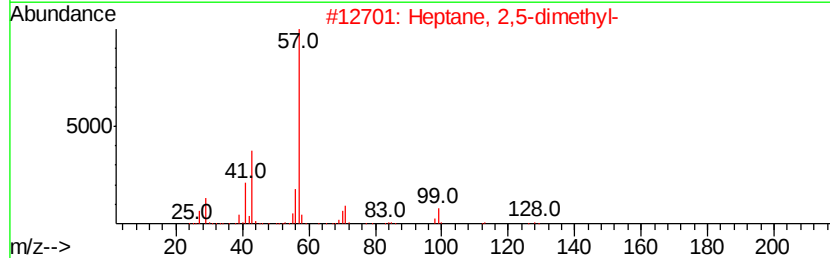
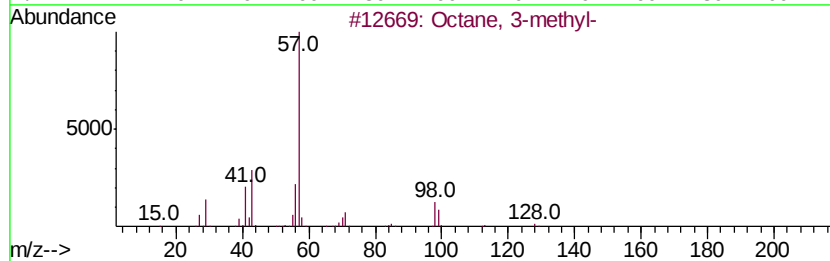
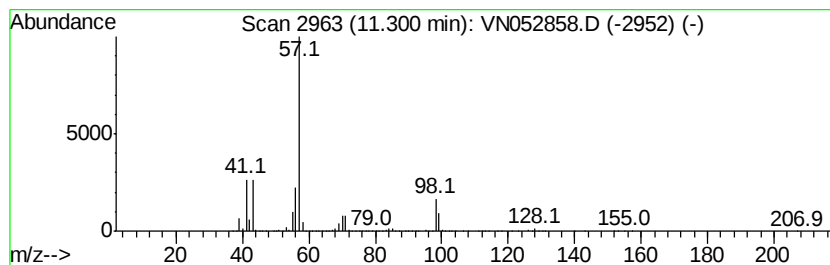
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Quant Title : SW846 8260

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

Peak Number 5 Octane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	169.22 ug/l	20978400	Chlorobenzene-d5	11.41

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		Decane, 2,5-dimethyl-	170	C12H26	017312-50-4	59
4		Undecane, 6-methyl-	170	C12H26	017302-33-9	53
5		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
056_BT-1-2

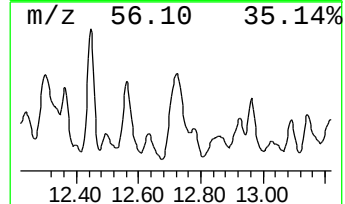
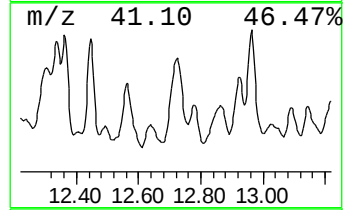
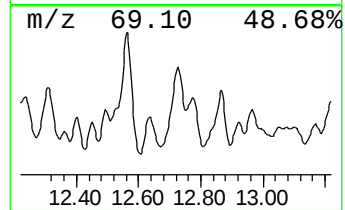
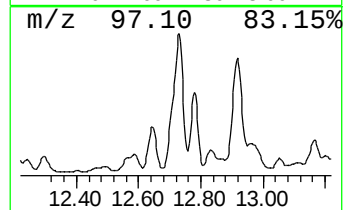
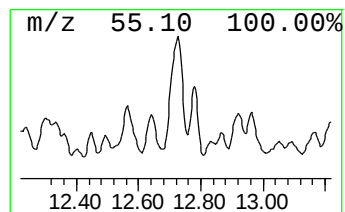
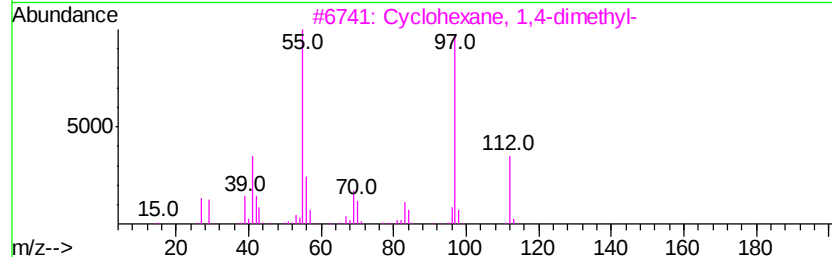
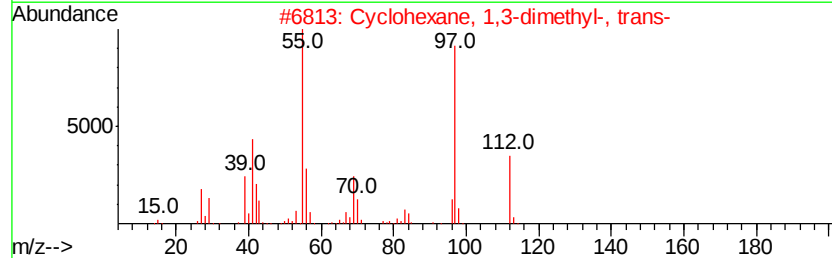
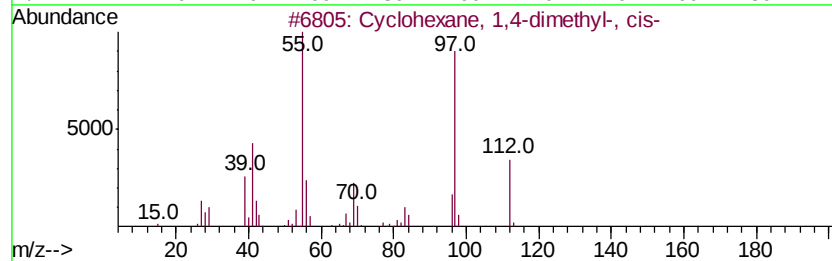
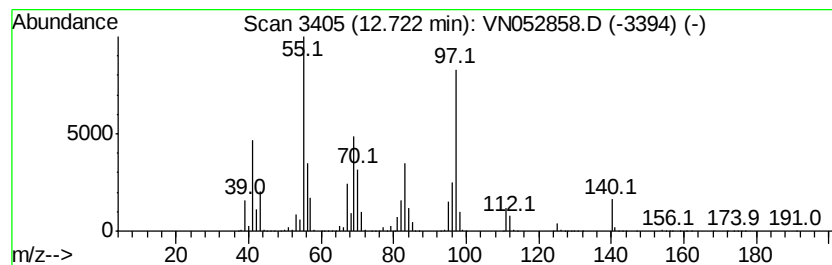
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Quant Title : SW846 8260

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

Peak Number 6 Cyclohexane, 1,4-dimethyl-,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	147.74 ug/l	11085600	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	62
2		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	49
3		Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	49
4		Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	49
5		Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
056_BT-1-2

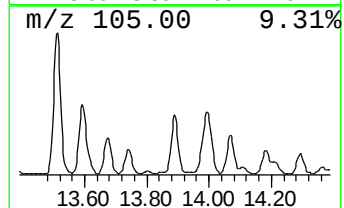
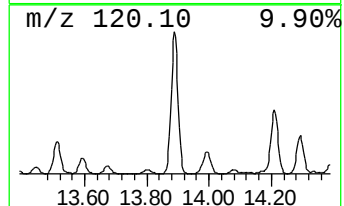
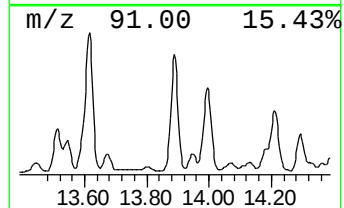
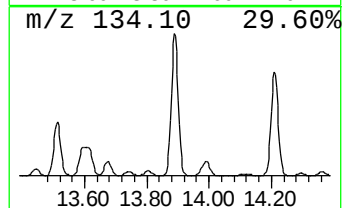
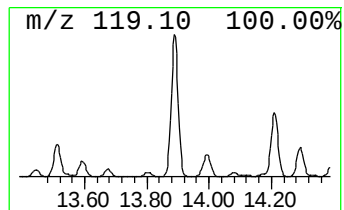
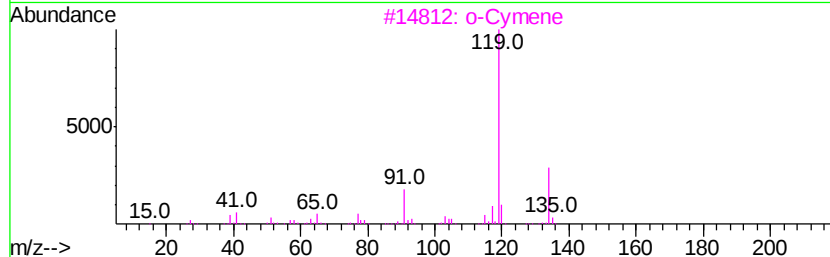
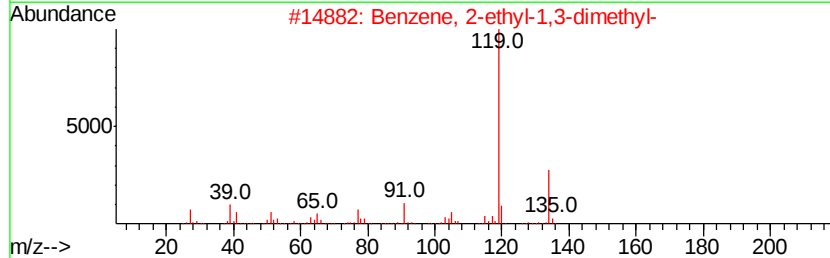
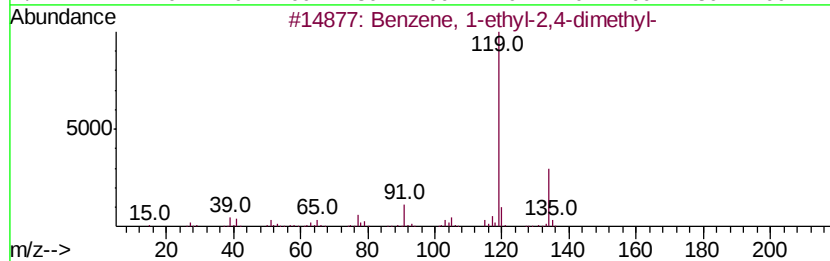
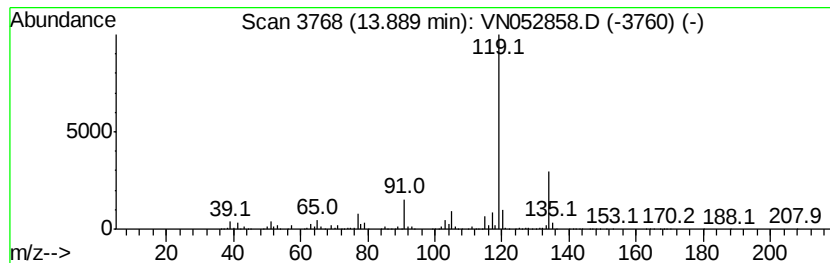
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Quant Title : SW846 8260

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

Peak Number 7 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	221.92 ug/l	16651900	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2		Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
3		o-Cymene	134	C10H14	000527-84-4	95
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

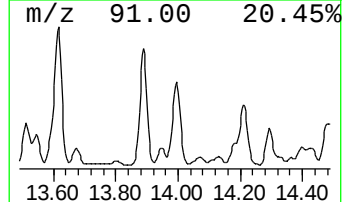
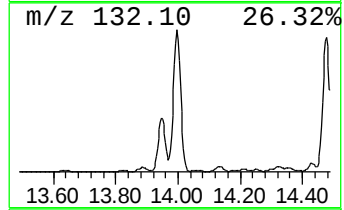
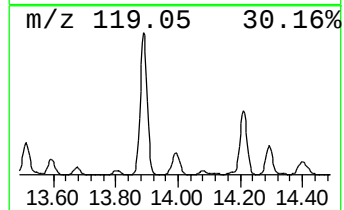
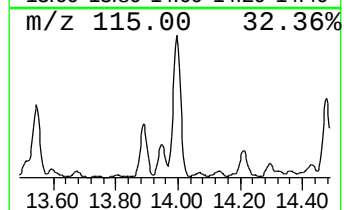
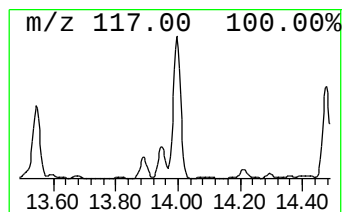
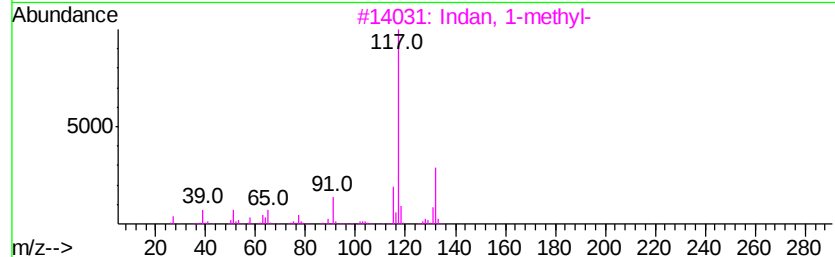
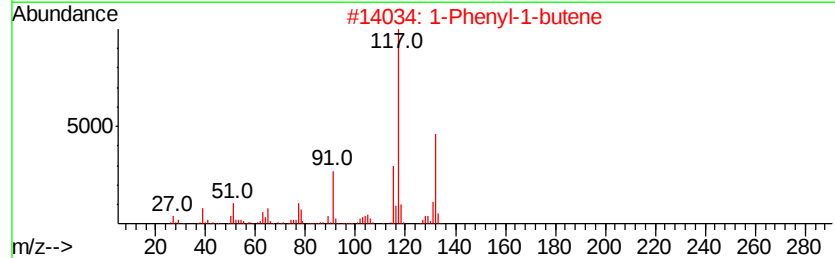
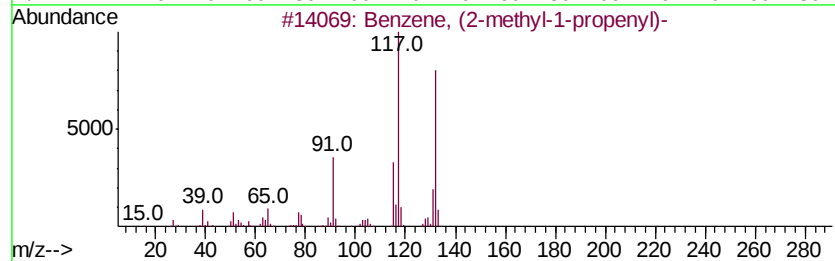
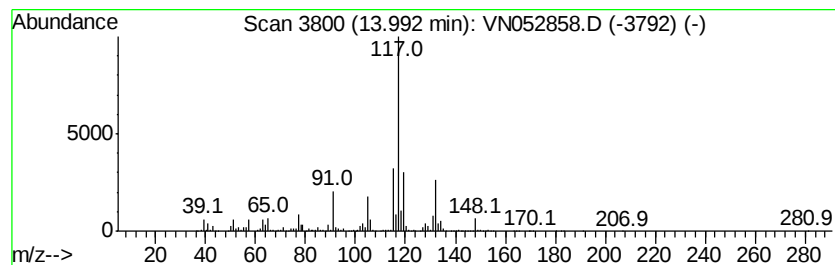
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ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzene, (2-methyl-1-propen... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	213.86 ug/l	16046800	1,4-Dichlorobenzene-d4	13.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, (2-methyl-1-propenyl)-	132 C10H12	000768-49-0 81
2		1-Phenyl-1-butene	132 C10H12	000824-90-8 81
3		Indan, 1-methyl-	132 C10H12	000767-58-8 76
4		Benzene, (2-methylcyclopropyl)-	132 C10H12	1000327-39-0 76
5		Benzene, 1-ethenyl-3-ethyl-	132 C10H12	007525-62-4 74



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
056_BT-1-2

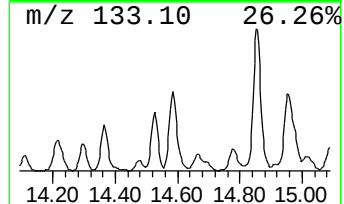
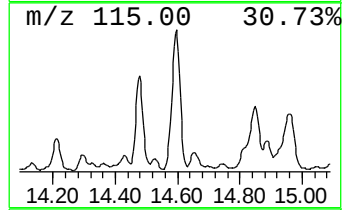
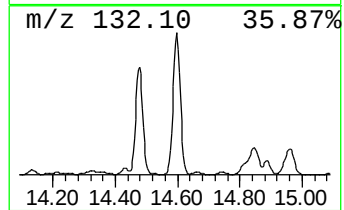
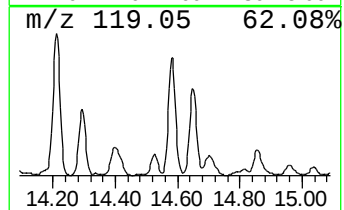
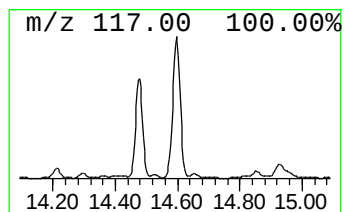
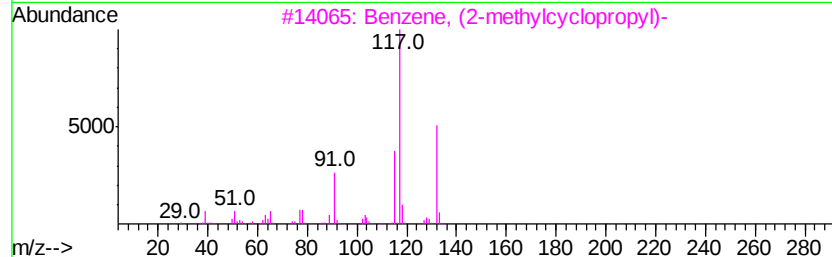
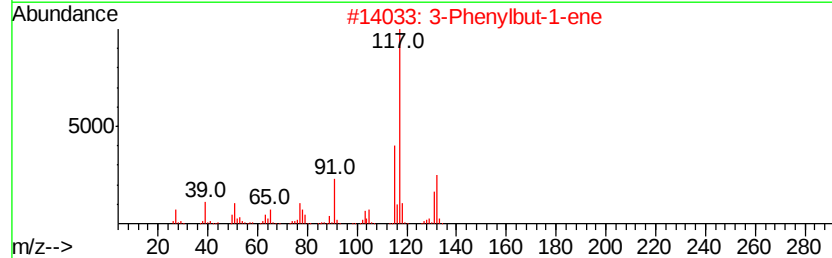
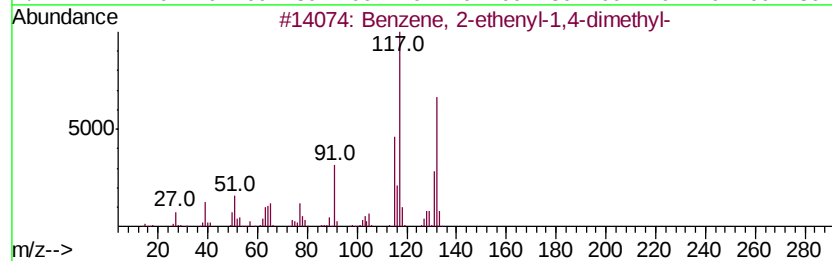
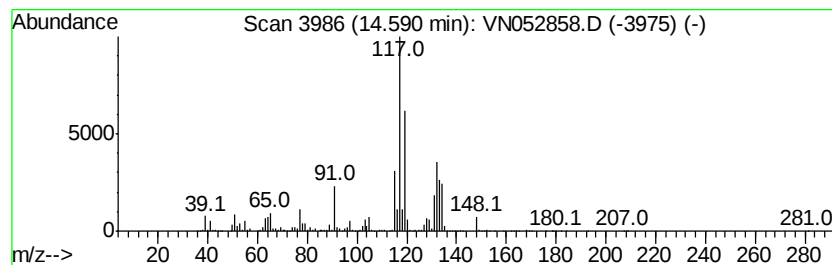
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Quant Title : SW846 8260

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

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	276.64 ug/l	20757800	1,4-Dichlorobenzene-d4	13.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	90
2		3-Phenylbut-1-ene	132	C10H12	000934-10-1	64
3		Benzene, (2-methylcyclopropyl)-	132	C10H12	1000327-39-0	60
4		Benzene, 2-butenyl-	132	C10H12	001560-06-1	58
5		1-Phenyl-1-butene	132	C10H12	000824-90-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
056_BT-1-2

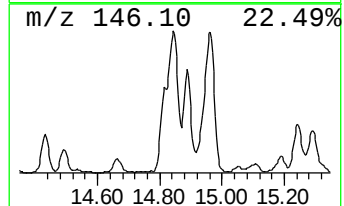
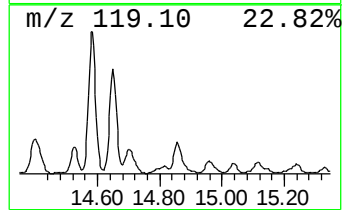
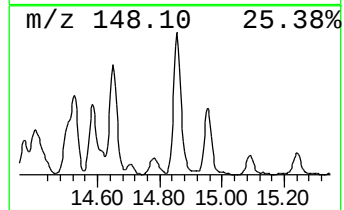
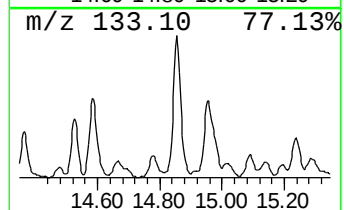
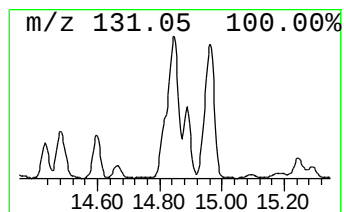
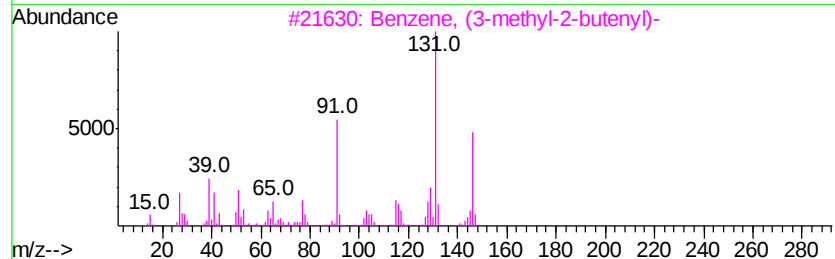
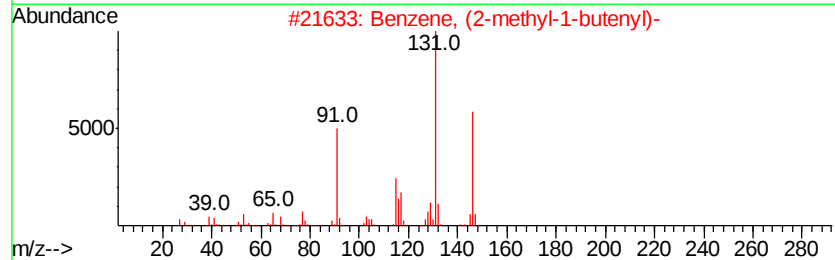
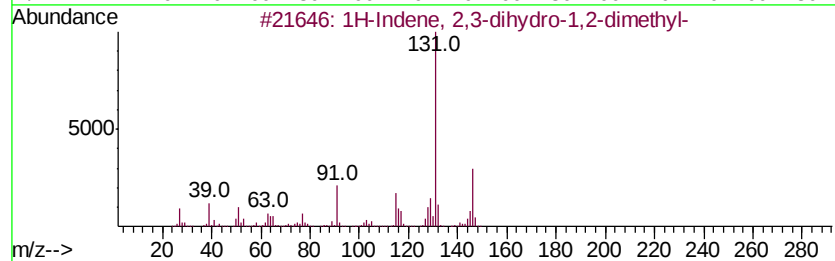
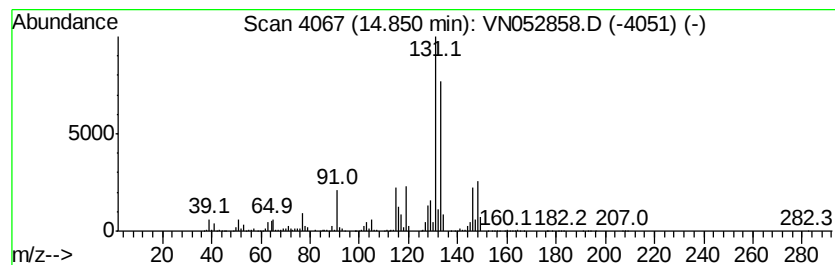
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Quant Title : SW846 8260

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

Peak Number 10 1H-Indene, 2,3-dihydro-1,2-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	152.76 ug/l	11462600	1,4-Dichlorobenzene-d4	13.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	90
2		Benzene, (2-methyl-1-butenyl)-	146	C11H14	056253-64-6	70
3		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64
4		Benzene, 1-methyl-3-(1-methyl-2-...	146	C11H14	052161-57-6	55
5		2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121318\
Data File : VN052858.D
Acq On : 13 Dec 2018 12:27
Operator : MD\SY
Sample : J6319-02
Misc : 5.16g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 8 Sample Multiplier: 28

Instrument :
MSVOA_N
ClientSampleId :
056_BT-1-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N121218W.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
Heptane, 2-methyl-	9.73	179.1	ug/l	35583700	2	8.59	9933490	50.0
Cyclohexane, ethyl-	10.95	145.4	ug/l	18021000	3	11.41	6198640	50.0
Octane, 2-methyl-	11.20	274.4	ug/l	34020300	3	11.41	6198640	50.0
Octane, 3-methyl-	11.30	169.2	ug/l	20978400	3	11.41	6198640	50.0
Cyclohexane, 1,4-...	12.72	147.7	ug/l	11085600	4	13.35	3751770	50.0
Benzene, 1-ethyl-...	13.89	221.9	ug/l	16651900	4	13.35	3751770	50.0
Benzene, (2-methy...	13.99	213.9	ug/l	16046800	4	13.35	3751770	50.0
Benzene, 2-etheny...	14.59	276.6	ug/l	20757800	4	13.35	3751770	50.0
1H-Indene, 2,3-di...	14.85	152.8	ug/l	11462600	4	13.35	3751770	50.0