

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070008.D
 Acq On : 11 Dec 2021 15:10
 Operator : JC/MD
 Sample : M4873-11
 Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A6-18-4.5

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: VN070008.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.995	369	375	389	rVB	153255	229095	1.22%	0.088%
2	3.392	508	523	547	rVB2	130614	327038	1.75%	0.126%
3	5.018	1102	1129	1130	rBV	118083	270044	1.44%	0.104%
4	5.082	1138	1153	1185	rVB4	429599	1454257	7.77%	0.558%
5	5.565	1305	1333	1371	rVB3	309591	1103069	5.90%	0.423%
6	6.080	1495	1525	1554	rBV3	363442	1145634	6.12%	0.440%
7	6.434	1645	1657	1685	rVB2	108451	325998	1.74%	0.125%
8	6.876	1797	1822	1842	rBV6	119060	387826	2.07%	0.149%
9	7.021	1849	1876	1895	rBV3	237788	726252	3.88%	0.279%
10	7.126	1896	1915	1935	rVV3	310783	884048	4.72%	0.339%
11	7.831	2164	2178	2196	rVB4	153703	381997	2.04%	0.147%
12	8.024	2223	2250	2252	rBV3	994133	1908818	10.20%	0.733%
13	8.163	2289	2302	2326	rVB3	748768	1943439	10.39%	0.746%
14	8.287	2328	2348	2368	rBV	1294720	2987410	15.97%	1.147%
15	8.434	2384	2403	2432	rBV	1094224	2693115	14.39%	1.034%
16	8.609	2432	2468	2491	rVV	2826725	8562209	45.76%	3.287%
17	8.697	2494	2501	2524	rVB4	270045	671707	3.59%	0.258%
18	8.818	2525	2546	2577	rVB2	1199652	2833818	15.15%	1.088%
19	8.963	2579	2600	2629	rBV2	3168536	7634198	40.80%	2.931%
20	9.121	2647	2659	2672	rVB2	197504	377727	2.02%	0.145%
21	9.196	2673	2687	2695	rBV3	150947	328986	1.76%	0.126%
22	9.453	2749	2783	2794	rBV2	1858810	4777413	25.53%	1.834%
23	9.507	2795	2803	2819	rVV	922665	1770008	9.46%	0.679%
24	9.588	2819	2833	2841	rVV	222717	474063	2.53%	0.182%
25	9.633	2842	2850	2864	rVV2	315058	587684	3.14%	0.226%
26	9.730	2865	2886	2902	rVV5	317282	823380	4.40%	0.316%
27	9.880	2926	2942	2964	rBV	2391942	5052038	27.00%	1.939%
28	9.974	2965	2977	2978	rBV2	535194	676323	3.61%	0.260%
29	10.014	2980	2992	3005	rVB	2887491	5480283	29.29%	2.104%
30	10.076	3005	3015	3024	rBV	1541327	2665247	14.24%	1.023%
31	10.215	3046	3067	3092	rBV2	1901797	4555001	24.34%	1.749%
32	10.317	3094	3105	3111	rBV6	214238	385863	2.06%	0.148%
33	10.368	3112	3124	3136	rVB2	1399580	2515355	13.44%	0.966%
34	10.440	3136	3151	3166	rBV	4734640	9321923	49.82%	3.579%
35	10.623	3204	3219	3233	rVB2	2245756	4447015	23.77%	1.707%
36	10.682	3233	3241	3251	rVB3	337728	502889	2.69%	0.193%

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37	10.784	3269	3279	3284	rBV4	276569	462417	2.47%	0.178%
38	10.864	3296	3309	3334	rVB8	858311	2639977	14.11%	1.013%
39	10.963	3336	3346	3359	rVB3	461145	871561	4.66%	0.335%
40	11.052	3360	3379	3391	rBV3	505645	1088187	5.82%	0.418%
41	11.154	3392	3417	3433	rBV3	794815	2297355	12.28%	0.882%
42	11.218	3435	3441	3446	rBV7	167896	219938	1.18%	0.084%
43	11.454	3521	3529	3538	rBV3	444519	664708	3.55%	0.255%
44	11.527	3545	3556	3582	rVB3	2210808	5066354	27.08%	1.945%
45	11.629	3582	3594	3616	rBV	1720771	3106622	16.60%	1.193%
46	11.747	3624	3638	3654	rBV	4744386	8434714	45.08%	3.238%
47	11.846	3664	3675	3694	rVB	4098636	7000055	37.41%	2.687%
48	11.953	3698	3715	3739	rVB2	8615366	18089537	96.68%	6.944%
49	12.283	3817	3838	3855	rBV	2627703	5812299	31.06%	2.231%
50	12.581	3939	3949	3959	rBV	1431976	2546503	13.61%	0.978%
51	12.734	3997	4006	4015	rVB	3005804	4590843	24.54%	1.762%
52	12.921	4065	4076	4087	rVB	2983326	4598634	24.58%	1.765%
53	12.983	4088	4099	4107	rBV	4809359	8103168	43.31%	3.111%
54	13.058	4119	4127	4142	rVB2	4766864	8618919	46.07%	3.309%
55	13.222	4176	4188	4204	rBV	3006271	5290426	28.28%	2.031%
56	13.369	4230	4243	4256	rVB	11699655	18710336	100.00%	7.183%
57	13.608	4326	4332	4339	rBV2	410766	542928	2.90%	0.208%
58	13.675	4347	4357	4364	rBV	4885469	8221462	43.94%	3.156%
59	13.839	4408	4418	4423	rBV	1794797	2762667	14.77%	1.061%
60	13.873	4424	4431	4439	rVV3	2682690	4182816	22.36%	1.606%
61	13.997	4467	4477	4489	rBV4	1578676	2433096	13.00%	0.934%
62	14.069	4496	4504	4516	rVB	1301555	1988708	10.63%	0.763%
63	14.134	4518	4528	4533	rBV	1562782	2507508	13.40%	0.963%
64	14.217	4548	4559	4572	rVB	5367033	8178282	43.71%	3.140%
65	14.327	4590	4600	4613	rVB4	2197764	3716177	19.86%	1.427%
66	14.461	4642	4650	4660	rBV3	695513	1141412	6.10%	0.438%
67	14.541	4672	4680	4688	rBV	2294407	3290646	17.59%	1.263%
68	14.579	4689	4694	4703	rVB	2028498	2571699	13.74%	0.987%
69	14.622	4703	4710	4719	rVB2	1164754	1476349	7.89%	0.567%
70	14.764	4757	4763	4770	rVB	512406	621915	3.32%	0.239%
71	14.812	4771	4781	4789	rBV	1856849	3200966	17.11%	1.229%
72	14.927	4808	4824	4837	rBV4	3325050	8456217	45.20%	3.246%
73	15.196	4915	4924	4953	rVB5	1756684	4344913	23.22%	1.668%
74	15.314	4956	4968	4983	rVB3	1247214	2747949	14.69%	1.055%
75	15.507	5031	5040	5053	rVB	1874639	3248222	17.36%	1.247%
76	15.807	5142	5152	5170	rVB	765826	1556396	8.32%	0.597%

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Integration Parameters: RTEINT.P

Integrator: RTE

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Sampling : 1

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Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M

Title : SW846 8260

77 16.620 5442 5455 5489 rVB 1598205 3876485 20.72% 1.488%

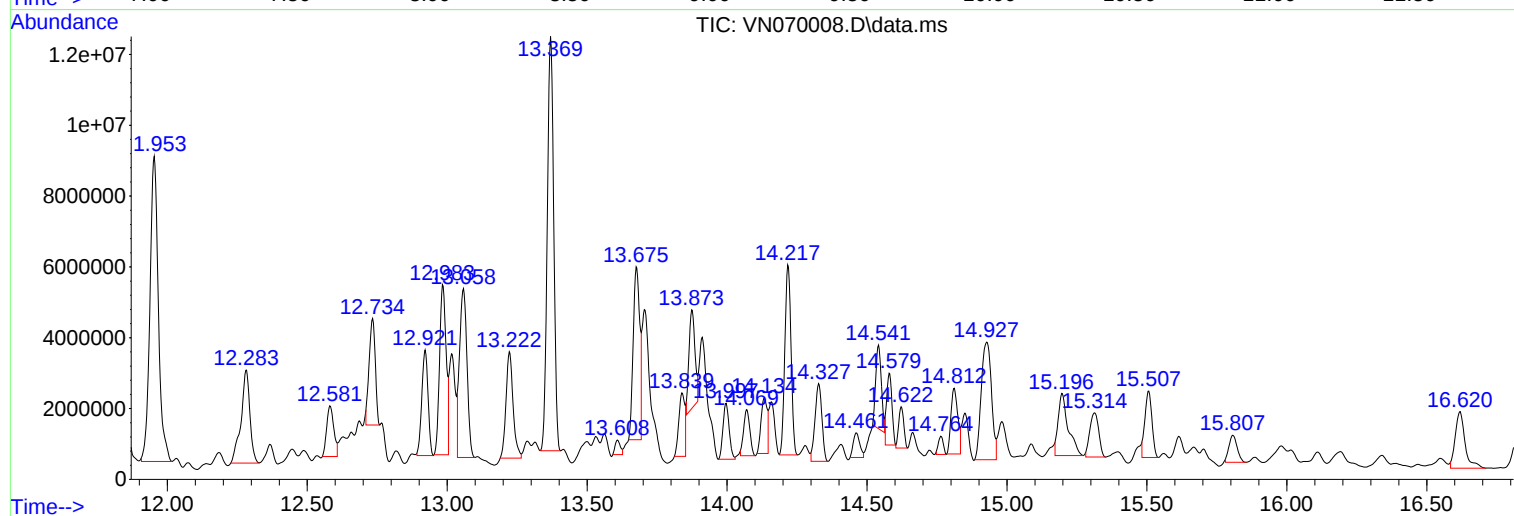
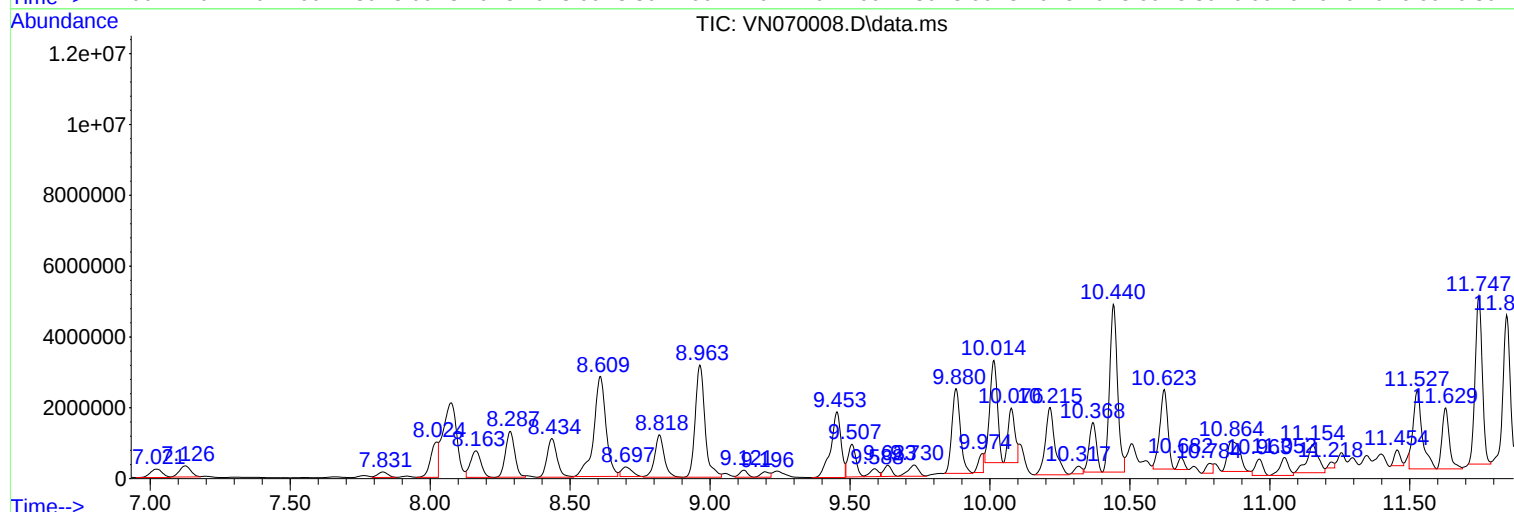
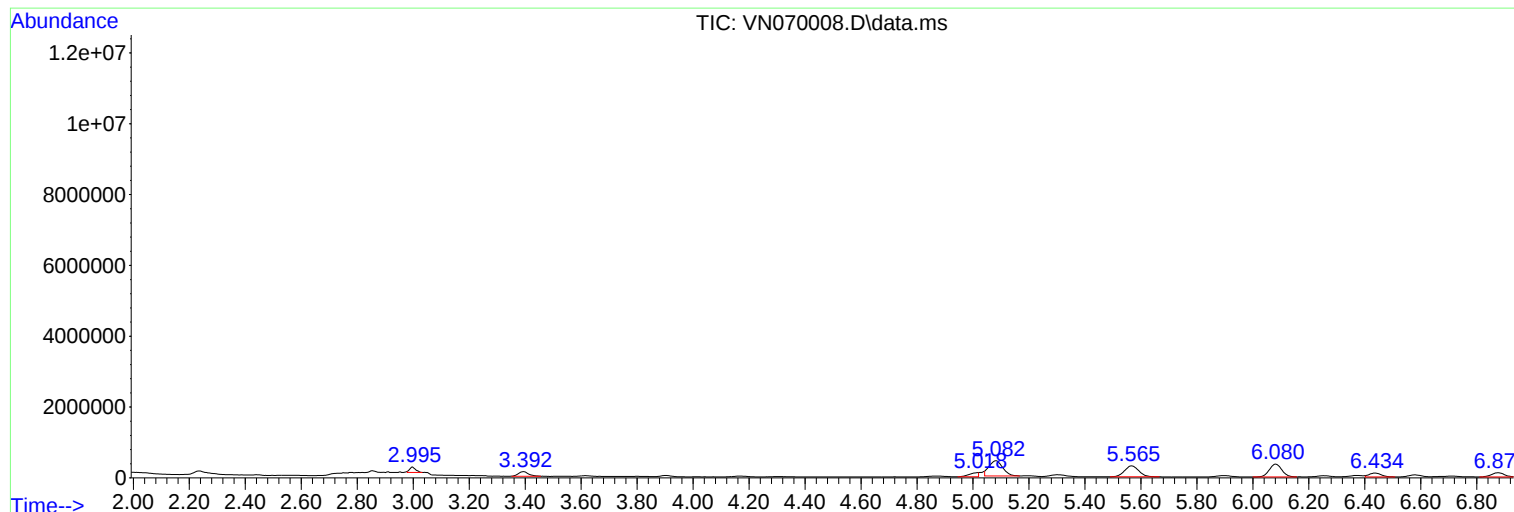
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Instrument :
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A6-18-4.5

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



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ALS Vial : 10 Sample Multiplier: 1

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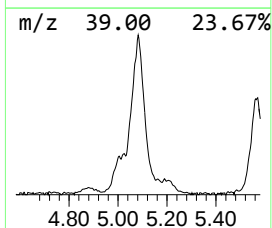
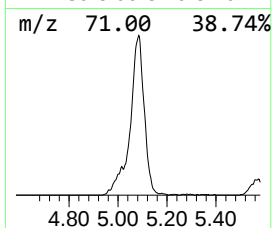
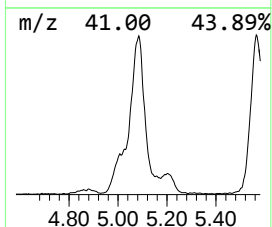
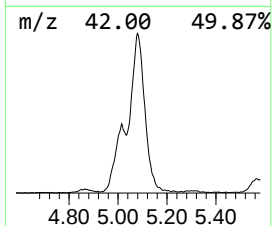
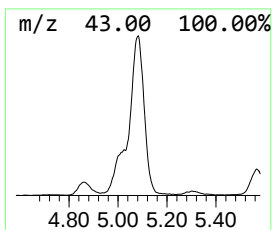
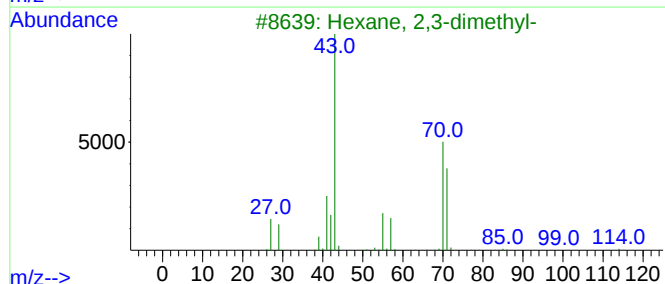
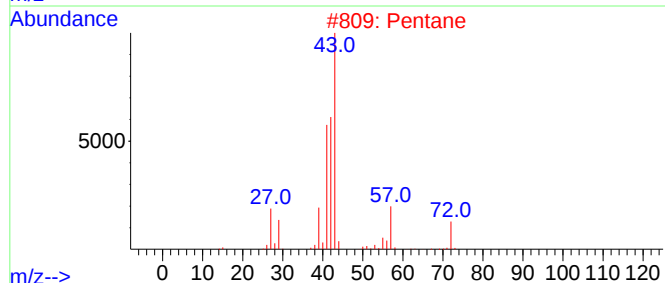
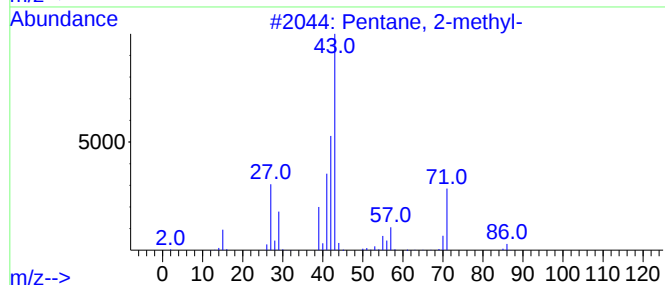
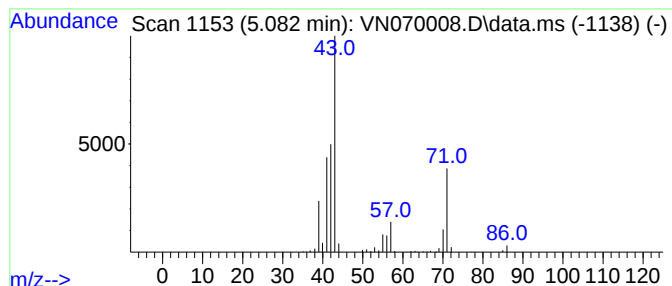
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.082	38.09 ug/l	1454260	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane	72	C5H12	000109-66-0	37
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28
4			C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	25
5			Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	25



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Instrument :
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ClientSampleId :
A6-18-4.5

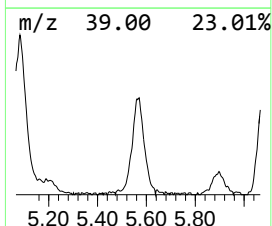
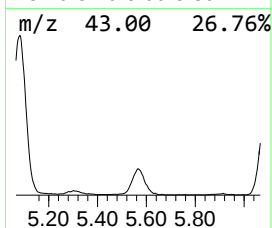
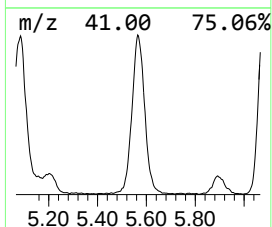
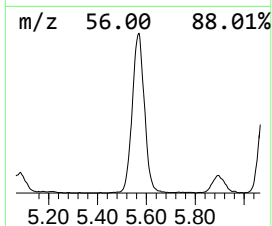
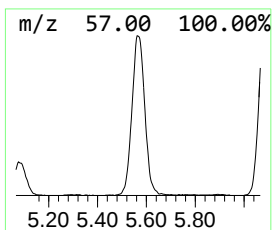
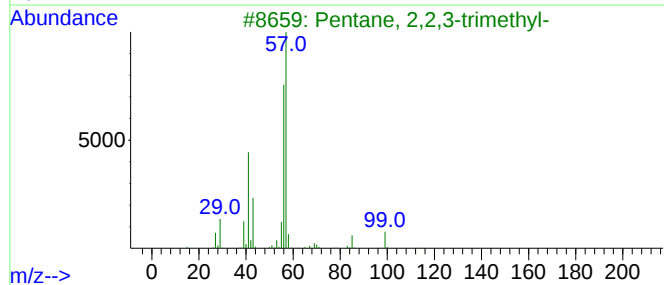
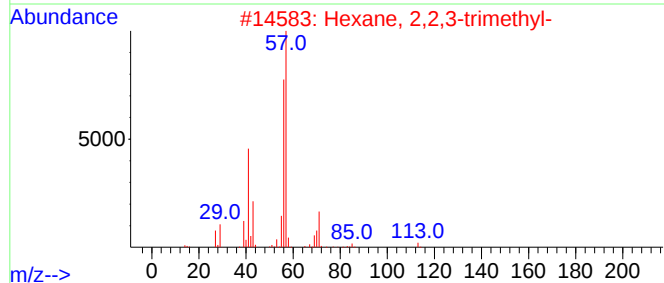
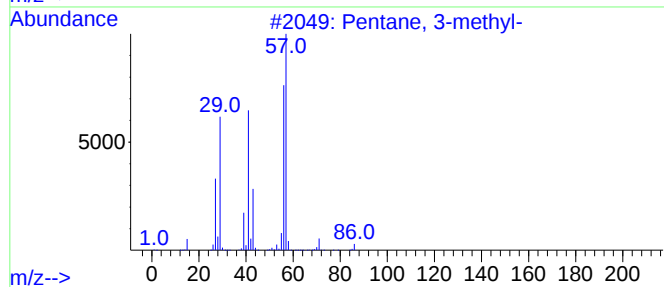
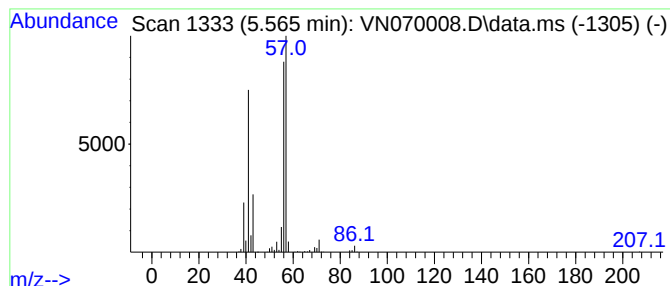
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.565	28.89 ug/l	1103070	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
3			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	78
4			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42



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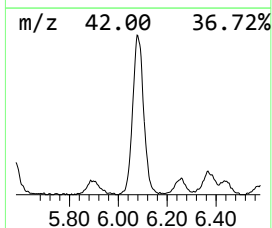
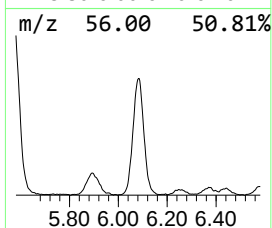
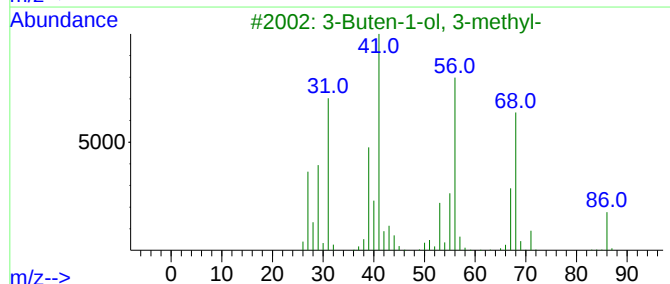
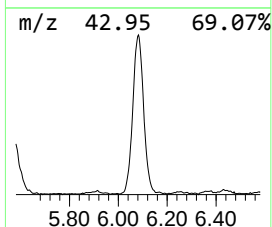
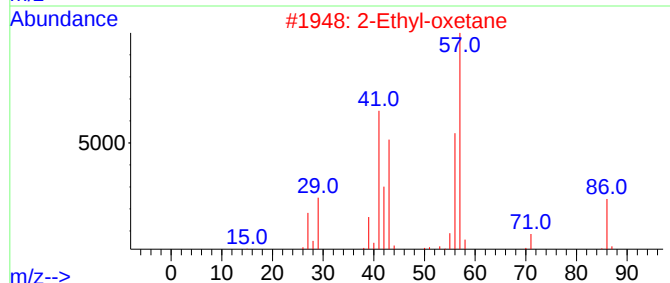
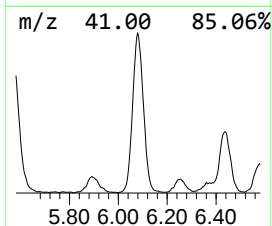
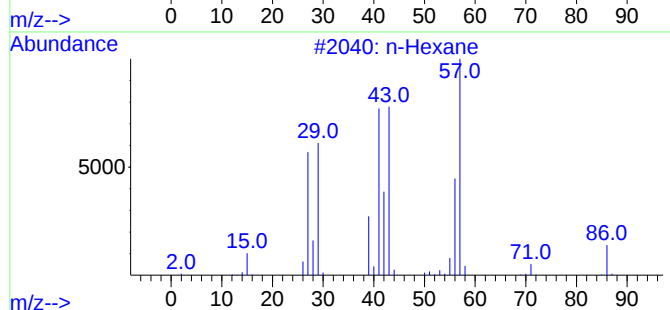
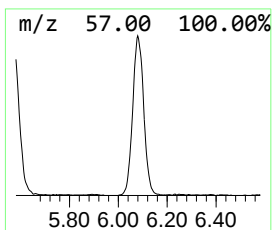
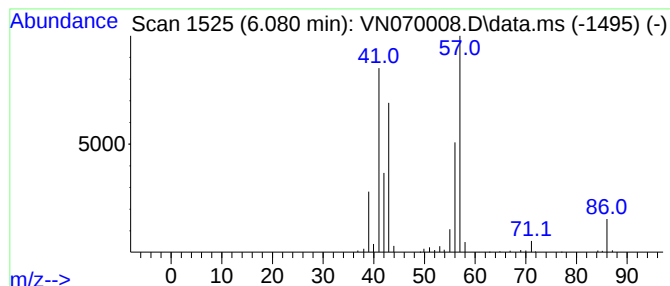
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 n-Hexane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.080	30.01 ug/l	1145630	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	91
3			3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	47
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	38
5			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	38



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A6-18-4.5

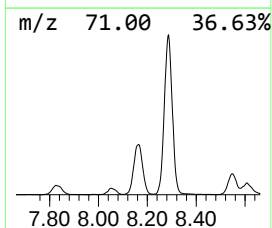
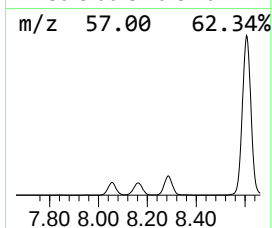
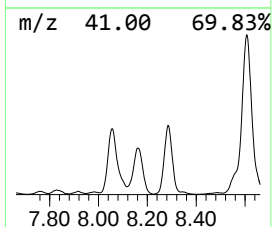
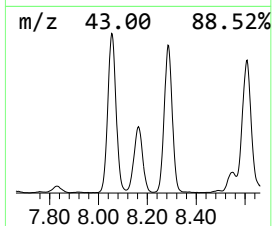
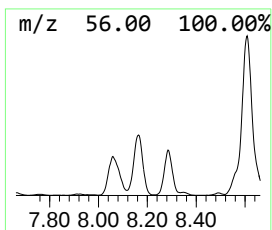
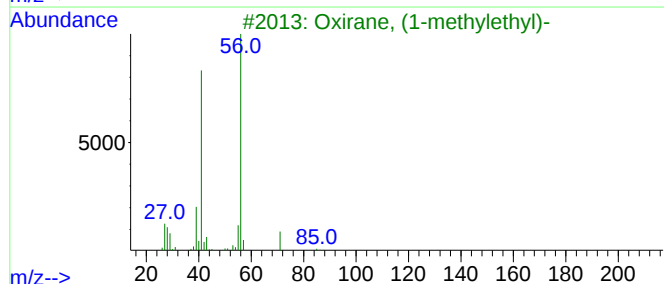
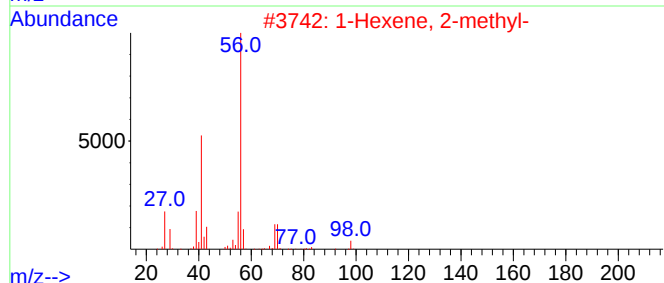
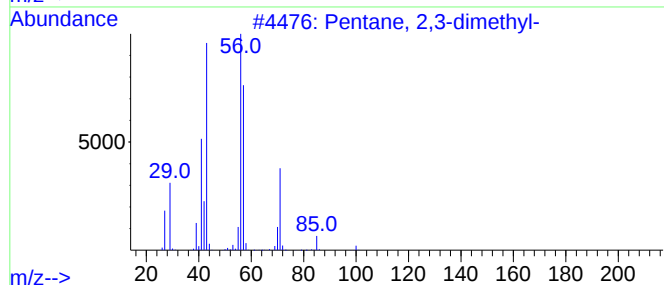
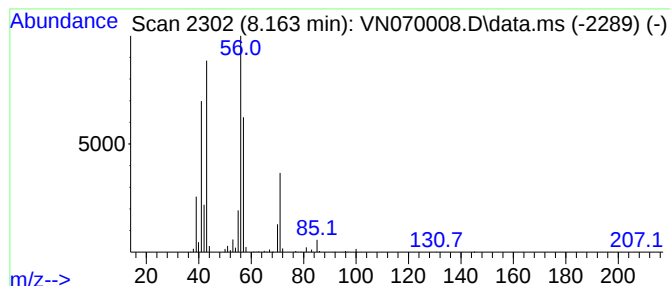
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.163	50.91 ug/l	1943440	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
3			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	37
4			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	37
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

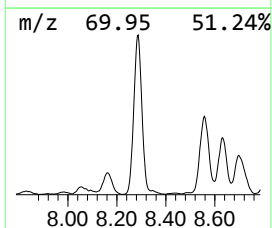
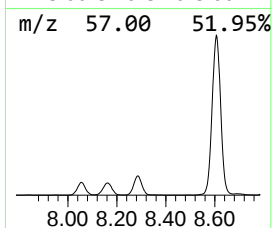
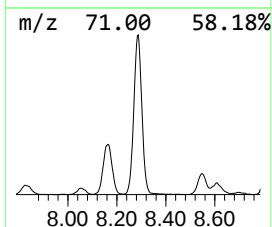
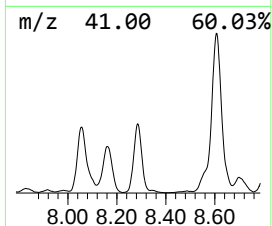
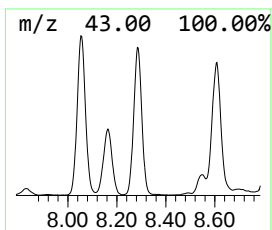
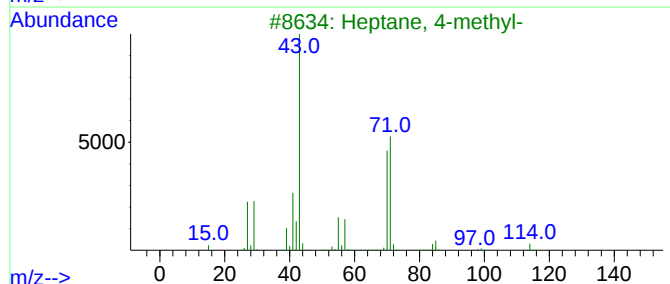
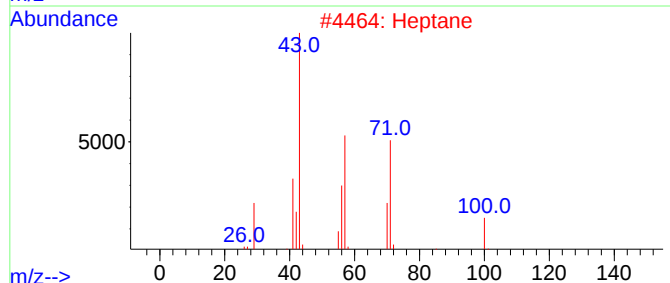
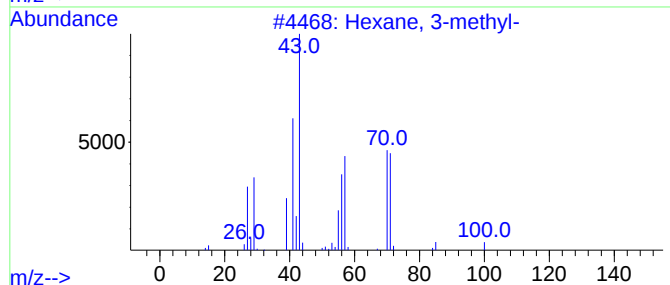
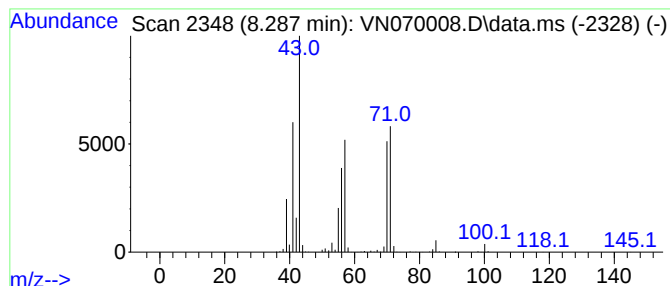
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.287	78.25 ug/l	2987410	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane	100	C7H16	000142-82-5	72
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	59
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	58
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

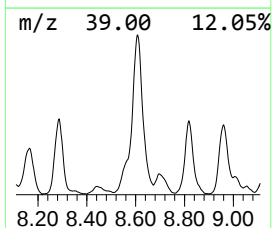
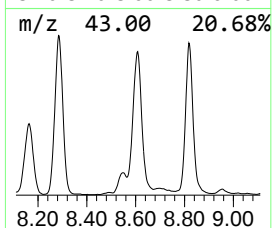
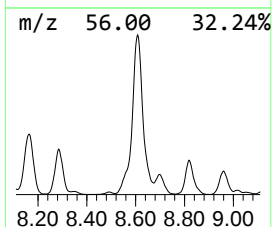
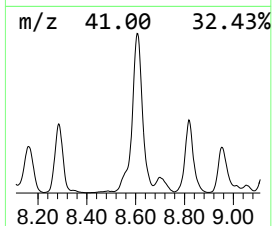
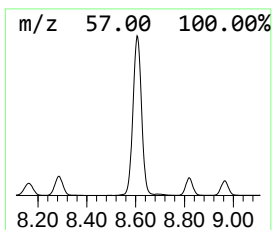
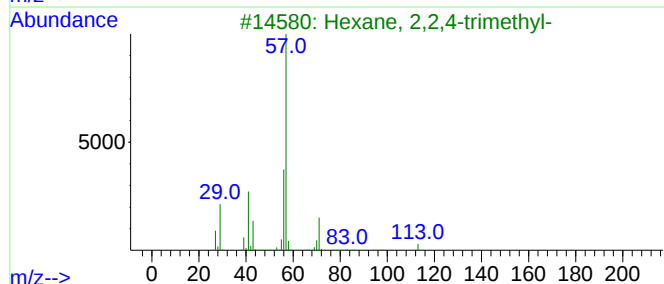
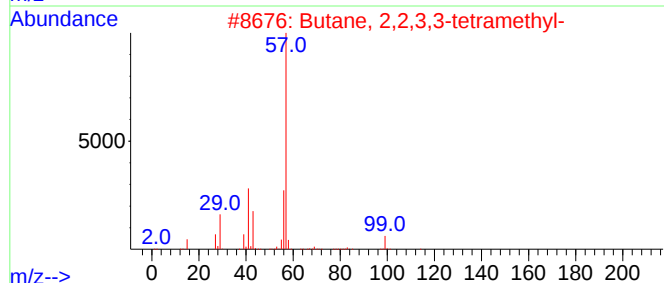
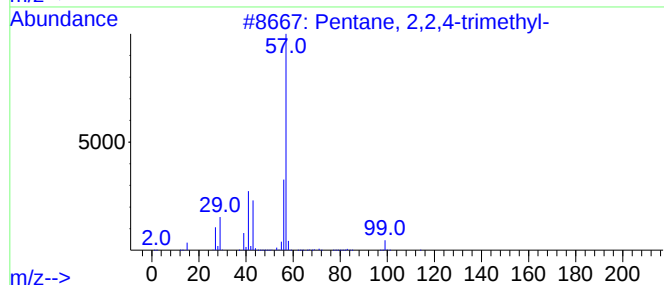
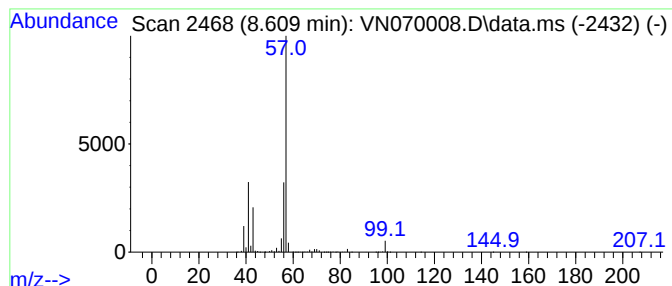
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.609	56.08 ug/l	8562210	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

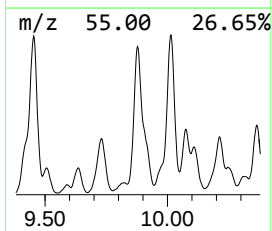
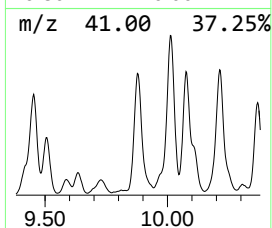
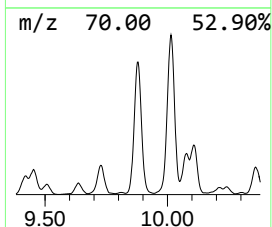
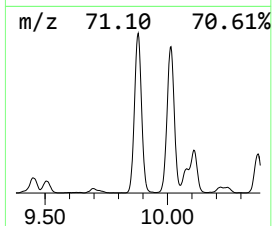
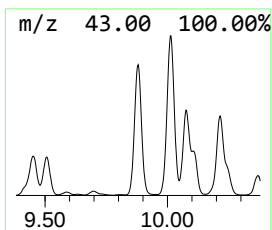
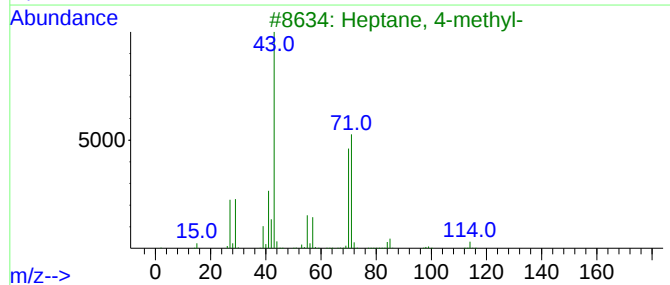
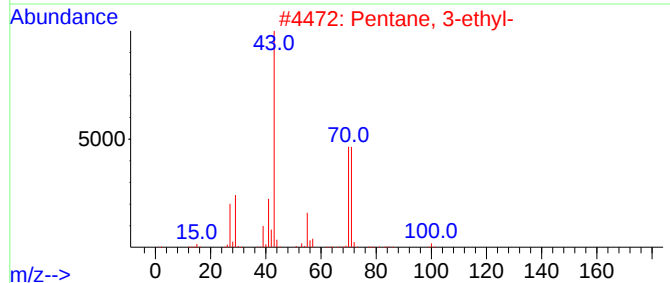
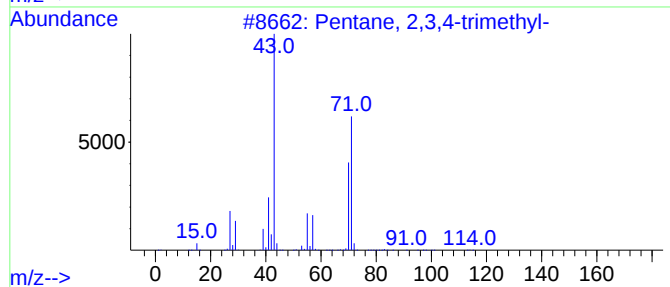
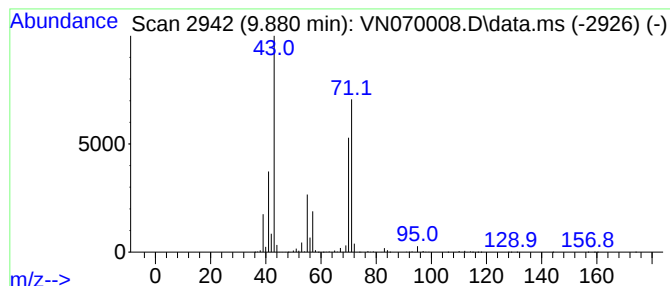
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	33.09 ug/l	5052040	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	74
4			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	64
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

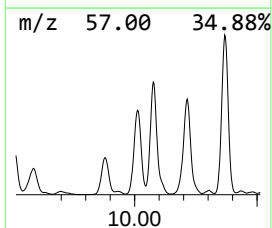
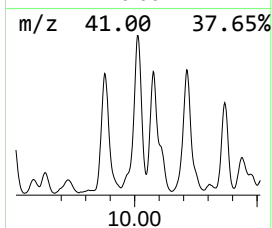
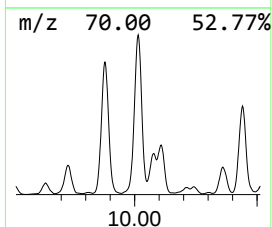
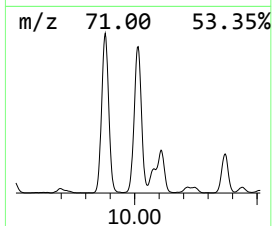
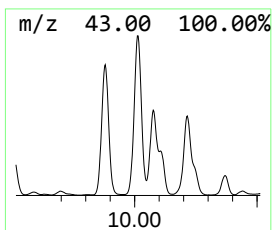
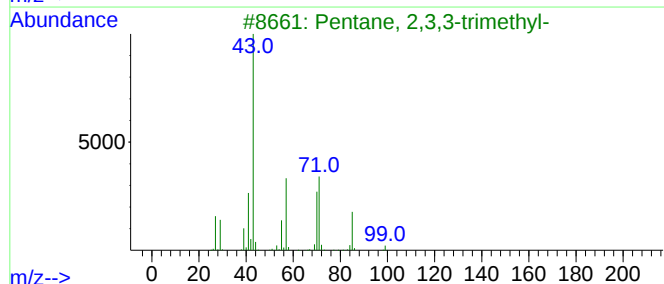
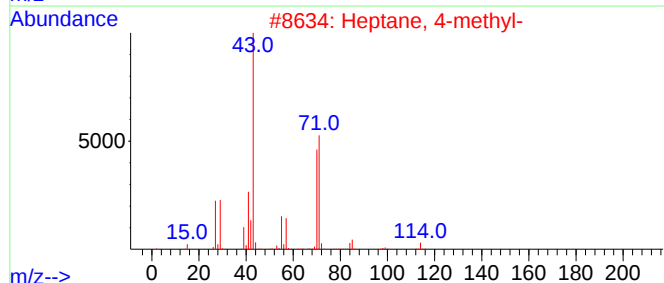
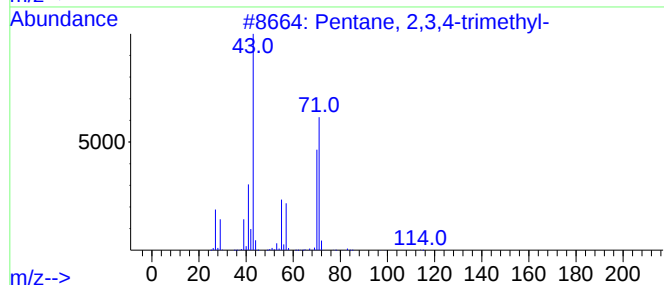
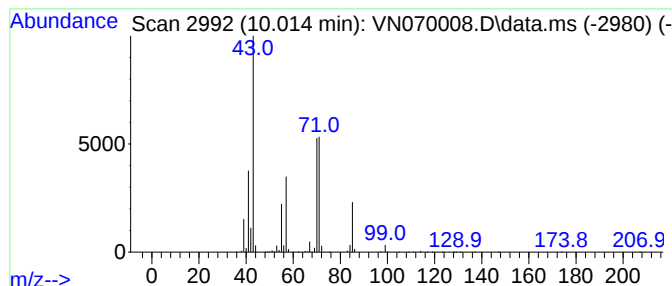
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Quant Title : SW846 8260

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

Peak Number 8 Heptane, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.014	35.89 ug/l	5480280	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	64
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

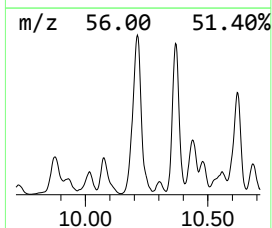
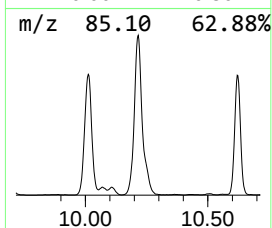
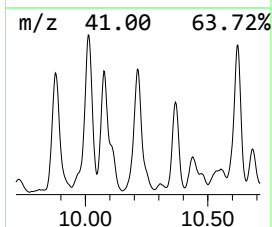
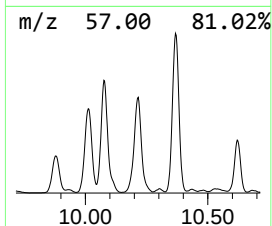
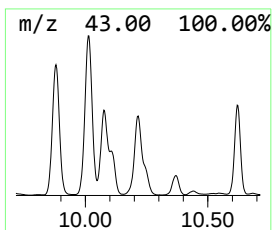
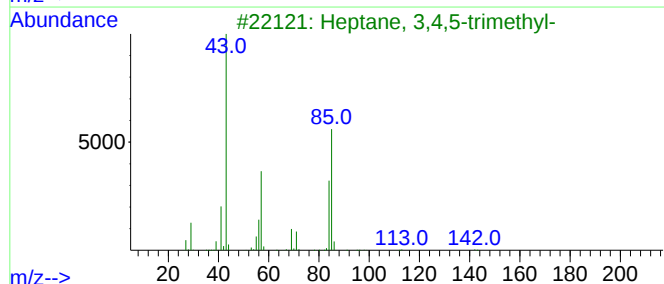
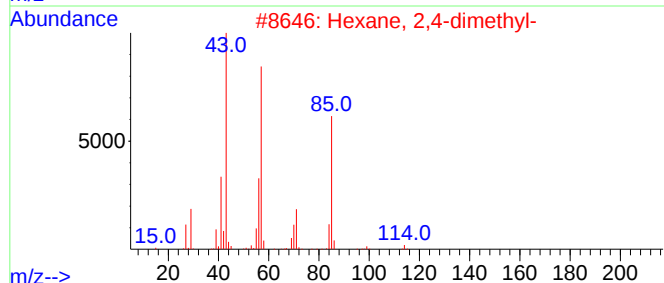
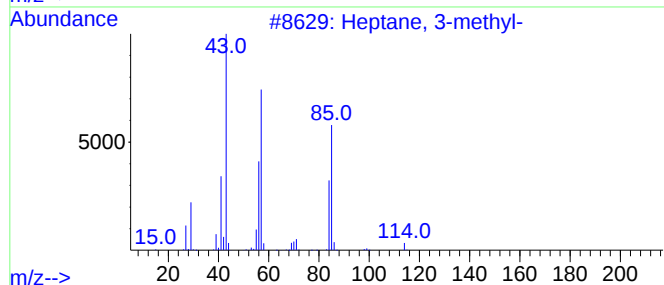
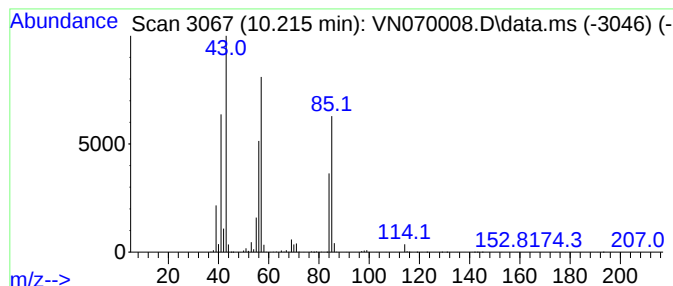
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Quant Title : SW846 8260

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

Peak Number 9 Heptane, 3-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.215	29.83 ug/l	4555000	1,4-Difluorobenzene	8.965

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3-methyl-	114	C8H18	000589-81-1	91
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	64
3			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
4			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	53
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A6-18-4.5

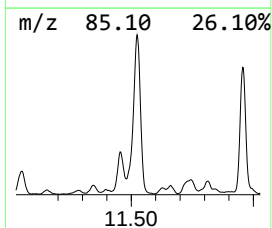
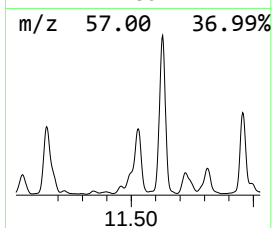
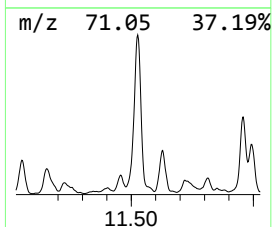
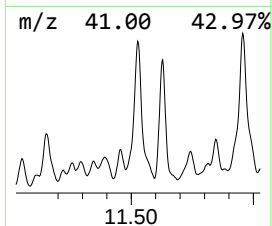
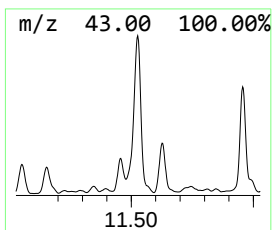
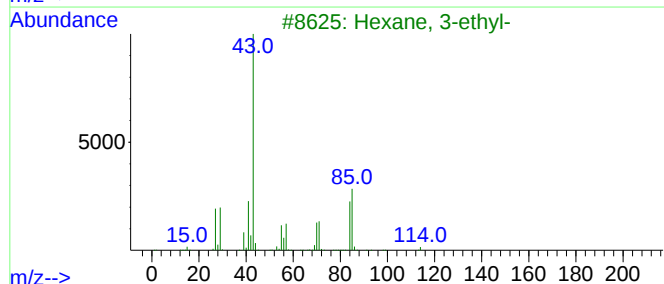
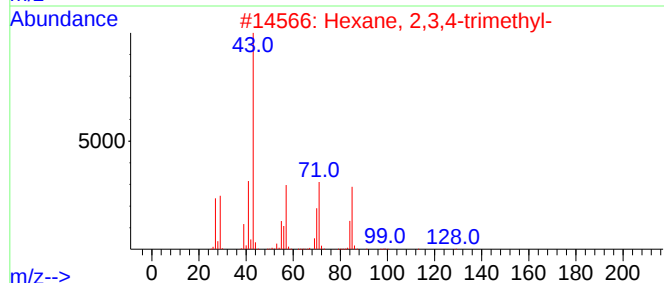
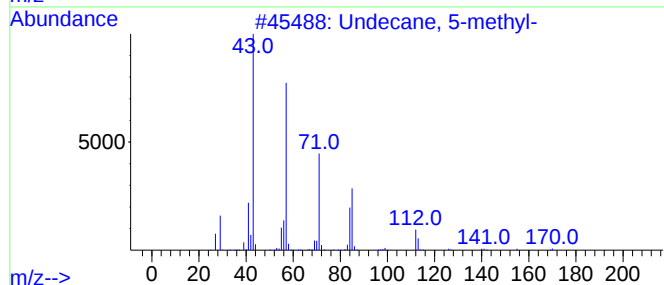
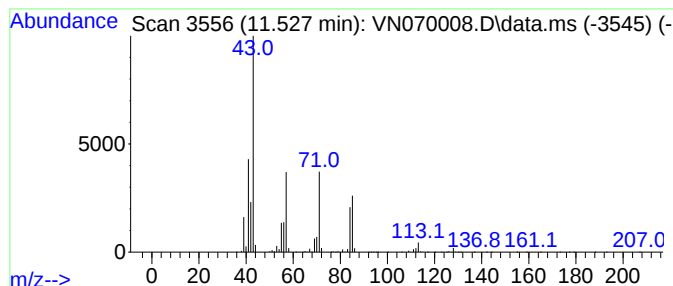
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Quant Title : SW846 8260

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

Peak Number 10 Undecane, 5-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.527	30.03 ug/l	5066350	Chlorobenzene-d5	11.747

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 5-methyl-	170	C12H26	001632-70-8	64
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
3			Hexane, 3-ethyl-	114	C8H18	000619-99-8	53
4			Octane, 2-methyl-	128	C9H20	003221-61-2	53
5			Octane, 4-methyl-	128	C9H20	002216-34-4	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

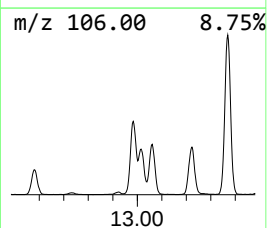
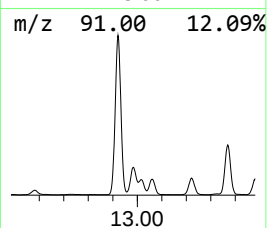
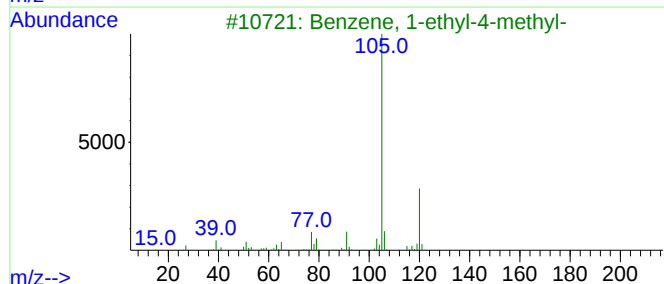
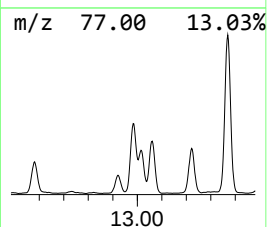
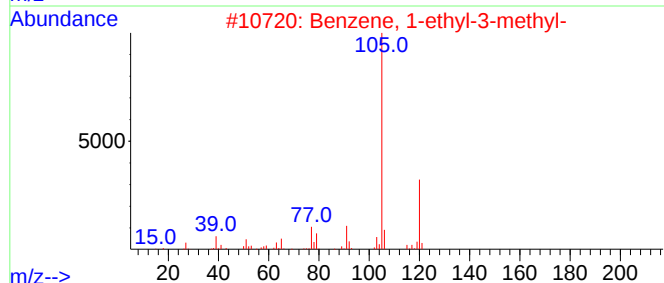
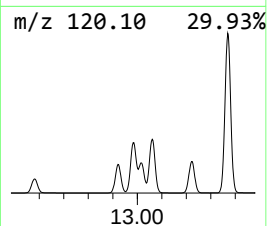
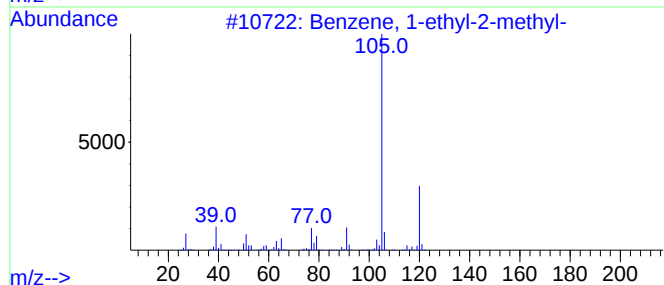
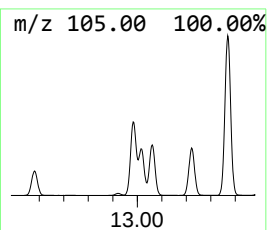
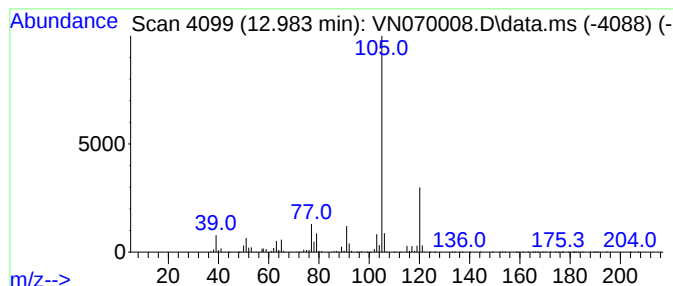
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Quant Title : SW846 8260

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

Peak Number 11 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	49.28 ug/l	8103170	1,4-Dichlorobenzene-d4	13.675

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	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

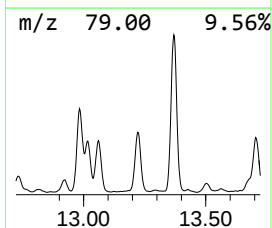
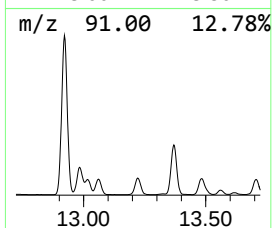
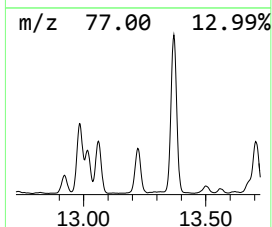
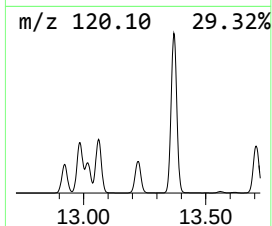
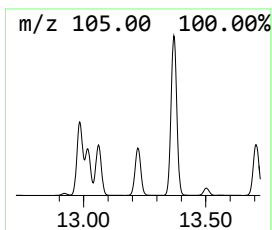
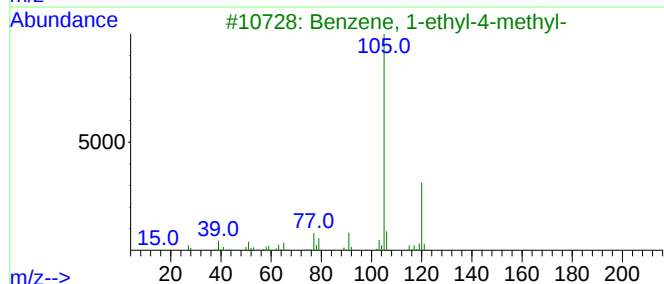
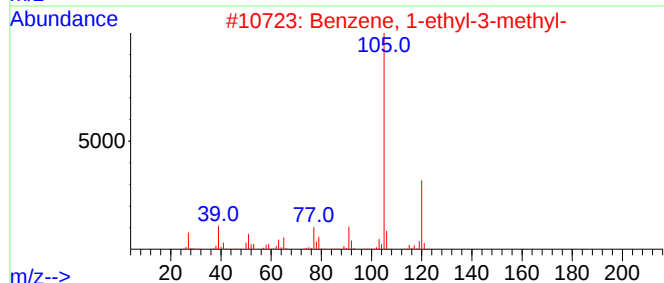
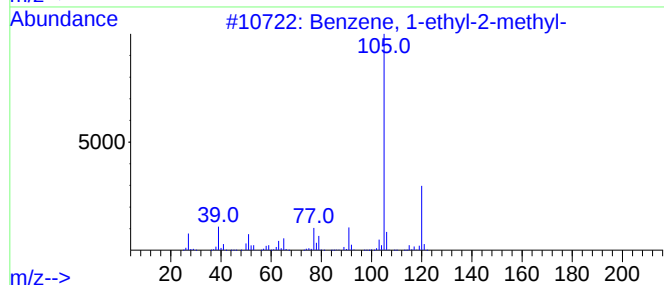
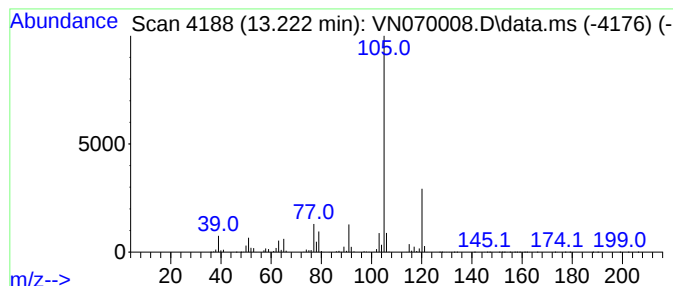
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Quant Title : SW846 8260

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

Peak Number 12 Benzene, 1-ethyl-3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	32.17 ug/l	5290430	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

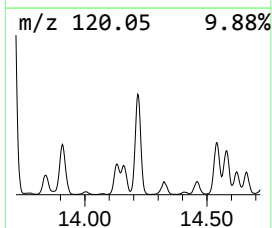
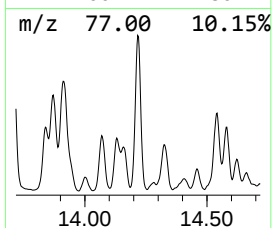
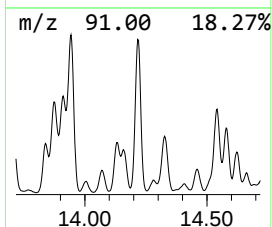
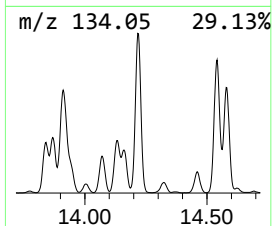
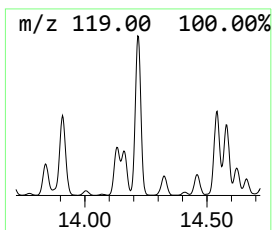
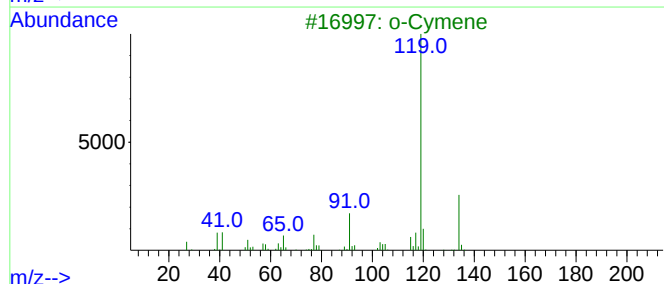
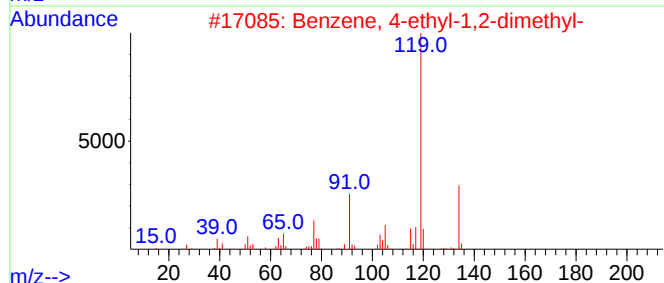
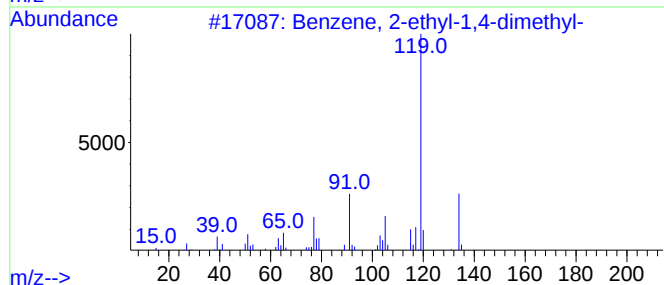
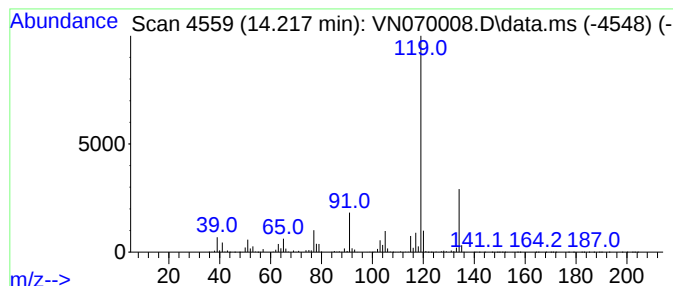
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Quant Title : SW846 8260

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

Peak Number 13 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.217	49.74 ug/l	8178280	1,4-Dichlorobenzene-d4	13.675

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

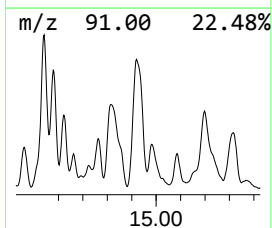
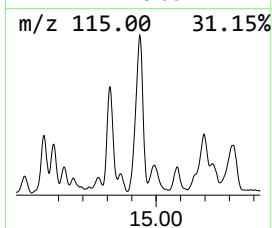
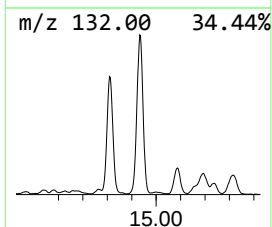
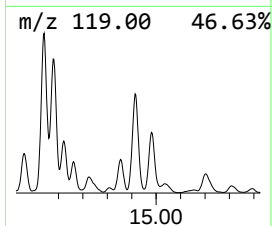
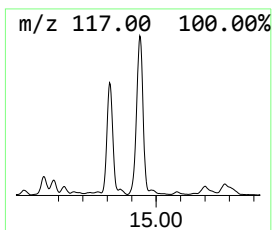
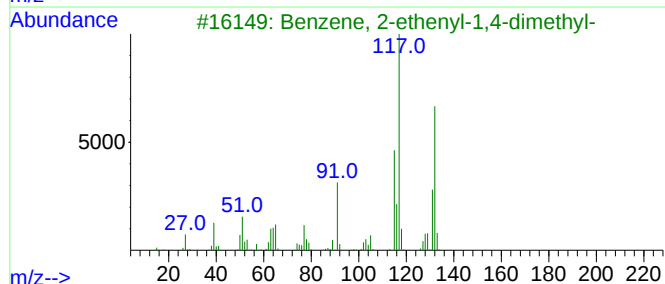
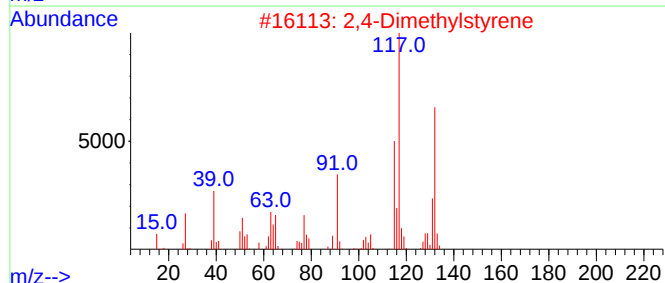
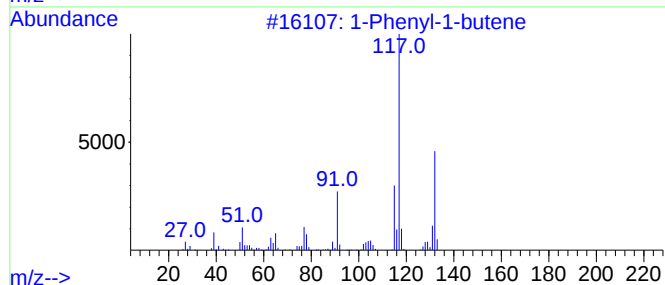
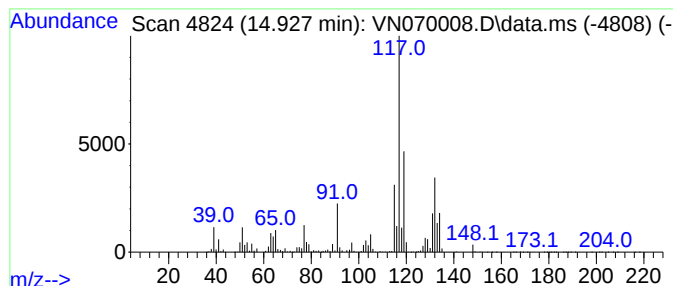
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Quant Title : SW846 8260

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

Peak Number 14 1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.927	51.43 ug/l	8456220	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	95
2			2,4-Dimethylstyrene	132	C10H12	002234-20-0	89
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	89
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	86
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070008.D
Acq On : 11 Dec 2021 15:10
Operator : JC/MD
Sample : M4873-11
Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A6-18-4.5

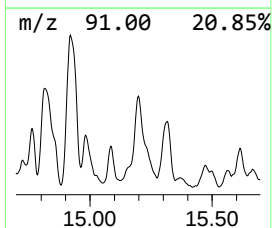
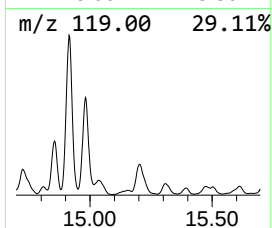
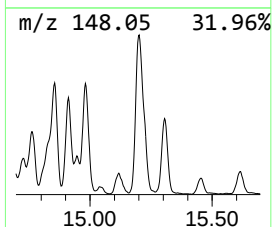
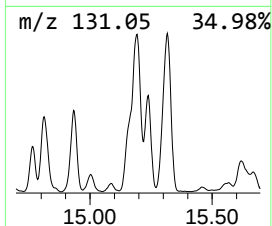
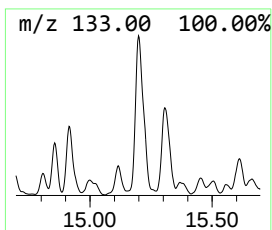
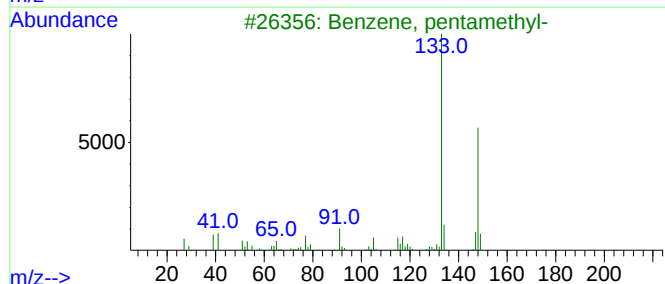
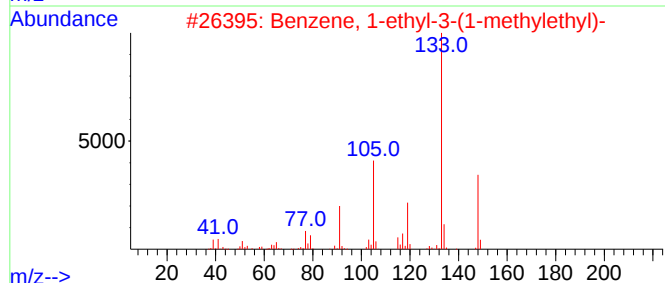
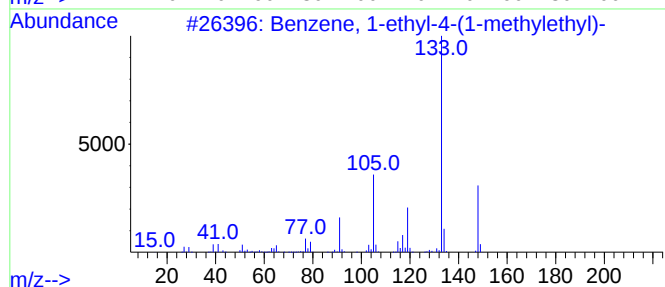
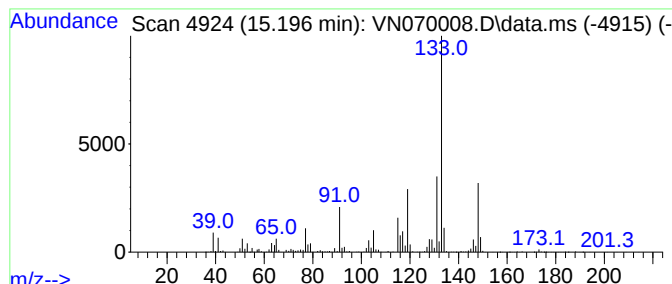
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 15 Benzene, 1-ethyl-4-(1-methy... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	26.42 ug/l	4344910	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	81
2			Benzene, 1-ethyl-3-(1-methylethyl)-	148	C11H16	004920-99-4	74
3			Benzene, pentamethyl-	148	C11H16	000700-12-9	68
4			1,5,6,7-Tetramethylbicyclo[3.2.0]...	148	C11H16	134329-46-7	64
5			Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	62



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070008.D
 Acq On : 11 Dec 2021 15:10
 Operator : JC/MD
 Sample : M4873-11
 Misc : 6.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A6-18-4.5

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

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2-methyl-	5.082	38.1	ug/l	1454260	1	8.080	1908820	50.0
Pentane, 3-methyl-	5.565	28.9	ug/l	1103070	1	8.080	1908820	50.0
n-Hexane	6.080	30.0	ug/l	1145630	1	8.080	1908820	50.0
Pentane, 2,3-di...	8.163	50.9	ug/l	1943440	1	8.080	1908820	50.0
Hexane, 3-methyl-	8.287	78.3	ug/l	2987410	1	8.080	1908820	50.0
Pentane, 2,2,4-...	8.609	56.1	ug/l	8562210	2	8.965	7634200	50.0
Pentane, 2,3,4-...	9.880	33.1	ug/l	5052040	2	8.965	7634200	50.0
Heptane, 4-methyl-	10.014	35.9	ug/l	5480280	2	8.965	7634200	50.0
Heptane, 3-methyl-	10.215	29.8	ug/l	4555000	2	8.965	7634200	50.0
Undecane, 5-met...	11.527	30.0	ug/l	5066350	3	11.747	8434710	50.0
Benzene, 1-ethy...	12.983	49.3	ug/l	8103170	4	13.675	8221460	50.0
Benzene, 1-ethy...	13.222	32.2	ug/l	5290430	4	13.675	8221460	50.0
Benzene, 2-ethy...	14.217	49.7	ug/l	8178280	4	13.675	8221460	50.0
1-Phenyl-1-butene	14.927	51.4	ug/l	8456220	4	13.675	8221460	50.0
Benzene, 1-ethy...	15.196	26.4	ug/l	4344910	4	13.675	8221460	50.0