

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
 Data File : VN070016.D
 Acq On : 11 Dec 2021 18:36
 Operator : JC/MD
 Sample : M4873-03 10X
 Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 A2-4-6.5

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: VN070016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.440	159	168	187	rVB2	163749	259998	1.98%	0.148%
2	3.113	401	419	460	rVB	1004442	2401318	18.33%	1.362%
3	3.497	545	562	594	rVB	449443	1116187	8.52%	0.633%
4	3.977	722	741	766	rVB4	77330	210674	1.61%	0.120%
5	4.237	817	838	853	rBV5	51528	161968	1.24%	0.092%
6	5.135	1121	1173	1210	rBV3	694715	3490700	26.64%	1.980%
7	5.613	1321	1351	1383	rBV3	479854	1672863	12.77%	0.949%
8	5.924	1447	1467	1495	rVB6	42591	134349	1.03%	0.076%
9	6.114	1508	1538	1566	rBV	434500	1336086	10.20%	0.758%
10	6.460	1655	1667	1693	rVB3	97990	294249	2.25%	0.167%
11	6.602	1697	1720	1738	rBV4	64951	198662	1.52%	0.113%
12	6.895	1805	1829	1858	rBV6	115409	367513	2.80%	0.209%
13	7.042	1858	1884	1902	rBV3	280263	853027	6.51%	0.484%
14	7.144	1903	1922	1945	rVV2	444006	1248443	9.53%	0.708%
15	7.842	2168	2182	2203	rVB3	130806	339232	2.59%	0.192%
16	8.024	2228	2250	2258	rBV	918111	2229688	17.02%	1.265%
17	8.083	2260	2272	2291	rVV2	2094150	5497209	41.95%	3.119%
18	8.174	2292	2306	2330	rVB	695144	1767348	13.49%	1.003%
19	8.297	2332	2352	2370	rBV	804915	1877134	14.33%	1.065%
20	8.442	2386	2406	2433	rBV2	1180894	3198576	24.41%	1.815%
21	8.617	2436	2471	2494	rVV	1708240	5279799	40.30%	2.996%
22	8.708	2497	2505	2526	rVV2	177336	436686	3.33%	0.248%
23	8.826	2530	2549	2577	rVB	643743	1517166	11.58%	0.861%
24	8.968	2582	2602	2632	rBV	2947413	6418828	48.99%	3.642%
25	9.126	2650	2661	2676	rVB4	84533	162902	1.24%	0.092%
26	9.247	2698	2706	2732	rVB4	86333	230843	1.76%	0.131%
27	9.459	2756	2785	2796	rBV2	972036	2432290	18.56%	1.380%
28	9.510	2797	2804	2822	rVV	426076	819704	6.26%	0.465%
29	9.593	2822	2835	2844	rVV	110776	237010	1.81%	0.134%
30	9.641	2845	2853	2866	rVV2	157177	287236	2.19%	0.163%
31	9.732	2866	2887	2903	rVB7	122690	319091	2.44%	0.181%
32	9.883	2928	2943	2965	rVB	1059391	2160411	16.49%	1.226%
33	10.017	2966	2993	3006	rBV2	1474976	3466520	26.46%	1.967%
34	10.081	3007	3017	3047	rVB4	661380	1774106	13.54%	1.007%
35	10.218	3048	3068	3094	rBV2	697299	1672545	12.76%	0.949%
36	10.322	3096	3107	3112	rBV5	78675	139738	1.07%	0.079%

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37	10.371	3113	3125	3137	rVB	909795	1584783	12.10%	0.899%
38	10.443	3137	3152	3169	rBV	4624902	8578818	65.47%	4.867%
39	10.625	3205	3220	3234	rVB2	751599	1505363	11.49%	0.854%
40	10.786	3269	3280	3296	rBV9	98938	269423	2.06%	0.153%
41	10.888	3297	3318	3336	rVB10	331978	994103	7.59%	0.564%
42	10.966	3337	3347	3360	rVB2	156834	285428	2.18%	0.162%
43	11.055	3360	3380	3392	rBV3	171138	352461	2.69%	0.200%
44	11.156	3394	3418	3434	rBV	262536	706774	5.39%	0.401%
45	11.457	3521	3530	3538	rBV3	154616	237014	1.81%	0.134%
46	11.529	3541	3557	3582	rVB3	696050	1654059	12.62%	0.938%
47	11.628	3583	3594	3616	rBV	537336	952530	7.27%	0.540%
48	11.746	3620	3638	3654	rBV	5049209	9101381	69.46%	5.164%
49	11.846	3663	3675	3695	rVB	2489014	4242449	32.38%	2.407%
50	11.956	3697	3716	3740	rBV2	3323411	6842950	52.23%	3.882%
51	12.184	3794	3801	3813	rVB7	129870	216318	1.65%	0.123%
52	12.280	3817	3837	3855	rVV2	633395	1561517	11.92%	0.886%
53	12.369	3863	3870	3880	rVB	238597	360700	2.75%	0.205%
54	12.581	3939	3949	3959	rBV2	353041	660655	5.04%	0.375%
55	12.731	3993	4005	4028	rVB	4244605	8152617	62.22%	4.625%
56	12.921	4051	4076	4087	rBV	1464763	2679898	20.45%	1.520%
57	12.983	4087	4099	4106	rBV	2537012	4237495	32.34%	2.404%
58	13.058	4119	4127	4142	rVB2	2948788	5232924	39.94%	2.969%
59	13.222	4173	4188	4204	rBV	1672575	3129866	23.89%	1.776%
60	13.286	4206	4212	4220	rVV2	168359	235377	1.80%	0.134%
61	13.369	4229	4243	4257	rBV	7945355	13102790	100.00%	7.434%
62	13.608	4326	4332	4339	rBV3	237004	315232	2.41%	0.179%
63	13.675	4345	4357	4398	rVB2	4845732	12162169	92.82%	6.900%
64	13.841	4408	4419	4422	rBV2	702464	979135	7.47%	0.556%
65	13.873	4423	4431	4438	rVV3	1883675	3313056	25.29%	1.880%
66	13.911	4440	4445	4466	rVB4	1974552	3730714	28.47%	2.117%
67	13.994	4467	4476	4488	rBV	1312970	1945791	14.85%	1.104%
68	14.072	4498	4505	4515	rVB	454798	644337	4.92%	0.366%
69	14.133	4518	4528	4532	rBV	1014900	1500514	11.45%	0.851%
70	14.217	4549	4559	4571	rVB	1789308	2714411	20.72%	1.540%
71	14.327	4590	4600	4612	rVB3	964384	1588945	12.13%	0.902%
72	14.463	4642	4651	4660	rBV3	354366	605412	4.62%	0.343%
73	14.541	4675	4680	4687	rVV2	504538	573243	4.37%	0.325%
74	14.579	4688	4694	4703	rVB	1049152	1420026	10.84%	0.806%
75	14.622	4704	4710	4718	rVB2	484163	591736	4.52%	0.336%
76	14.764	4757	4763	4771	rVB	294563	344274	2.63%	0.195%

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77	14.812	4771	4781	4788	rBV4	818046	1369694	10.45%	0.777%
78	14.850	4790	4795	4807	rVB3	921198	1327033	10.13%	0.753%
79	14.930	4809	4825	4837	rBV5	1337498	3318687	25.33%	1.883%
80	15.198	4917	4925	4953	rVB5	643258	1602030	12.23%	0.909%
81	15.507	5031	5040	5053	rVB	809908	1385942	10.58%	0.786%
82	16.620	5442	5455	5491	rVB	757514	1934402	14.76%	1.098%

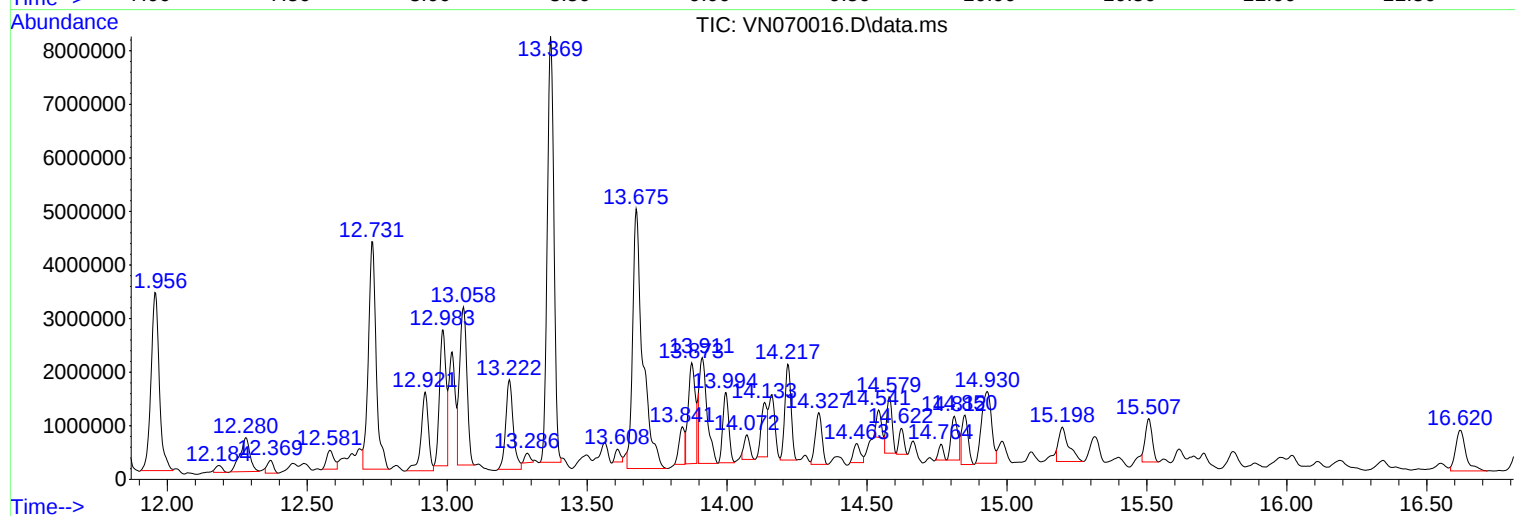
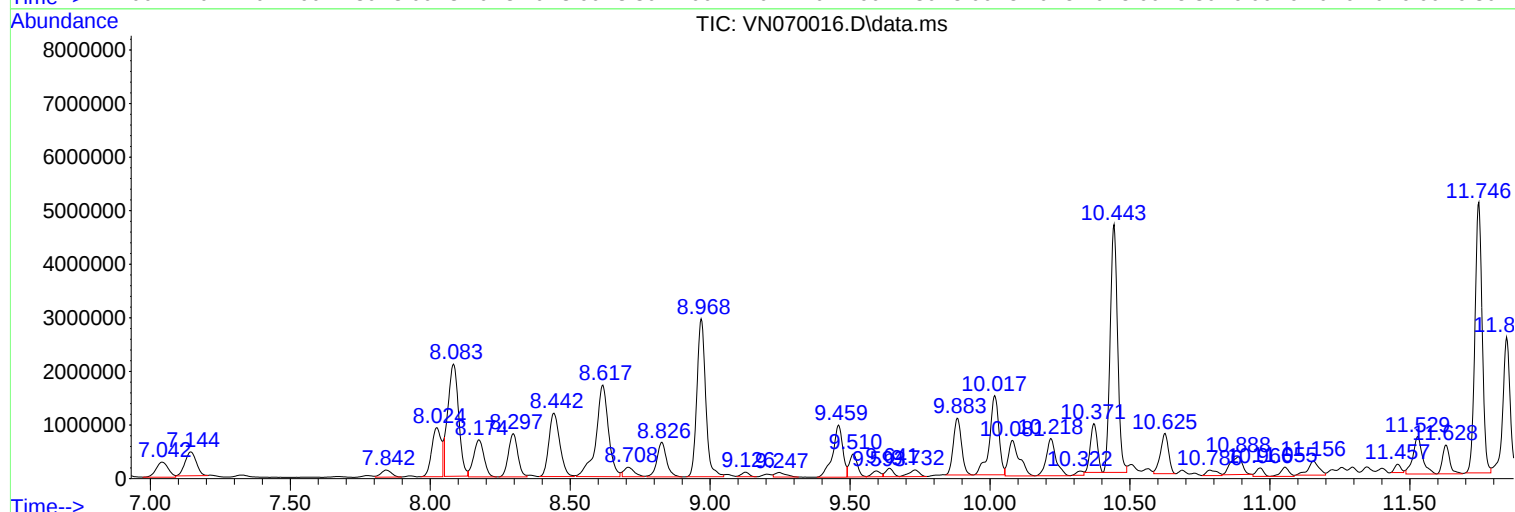
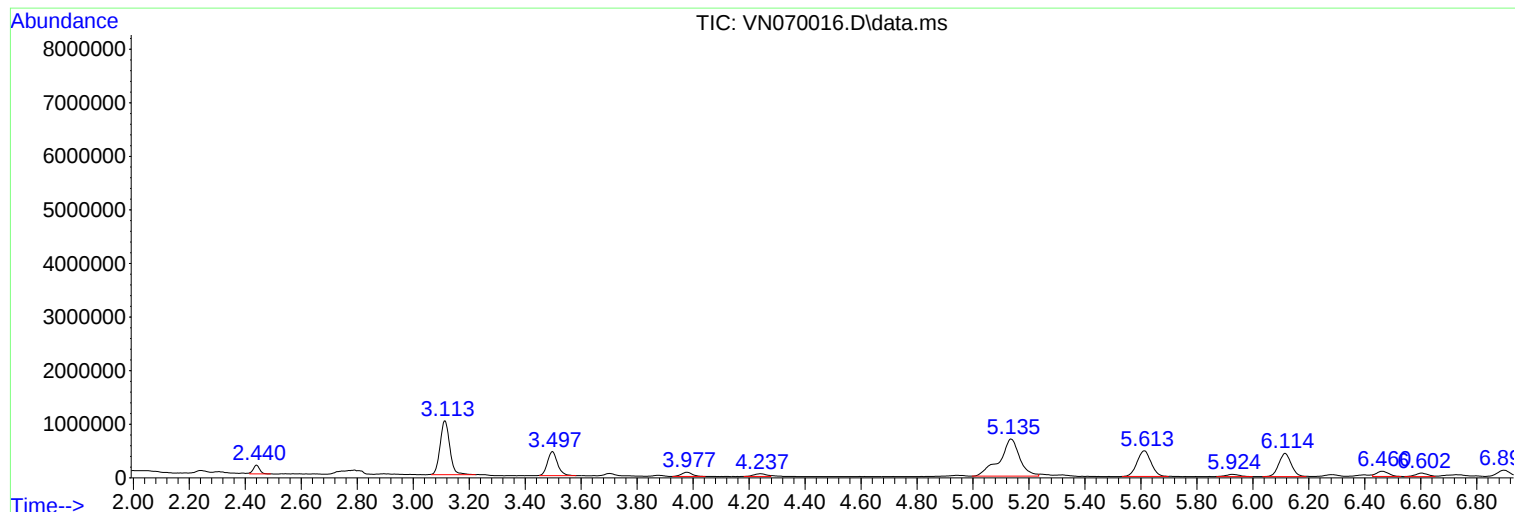
Sum of corrected areas: 176254575

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Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

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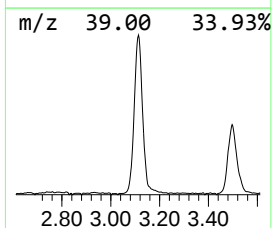
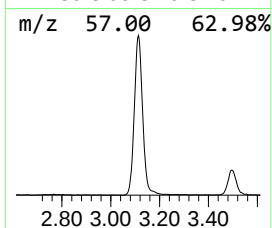
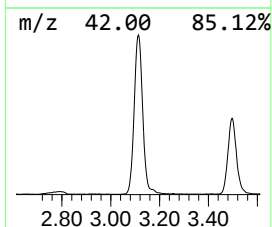
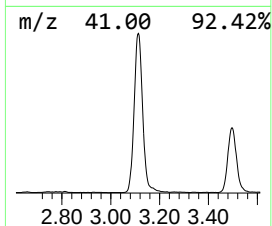
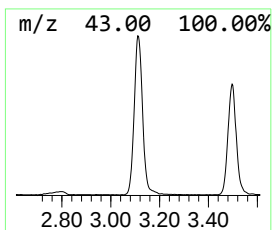
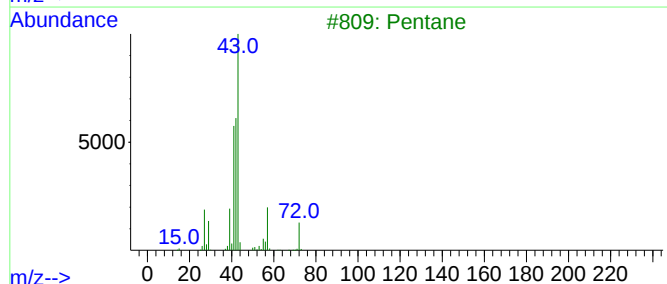
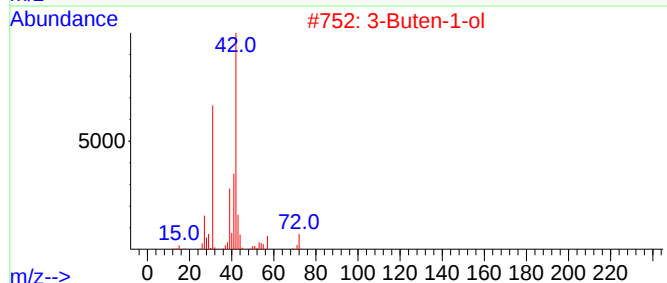
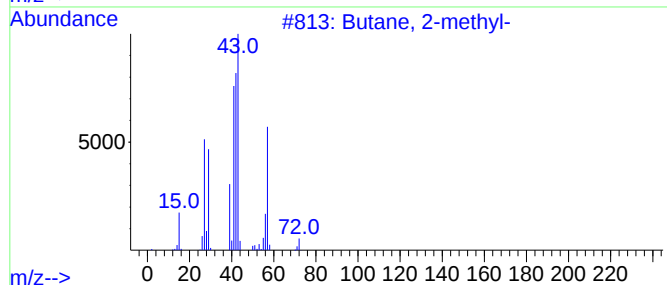
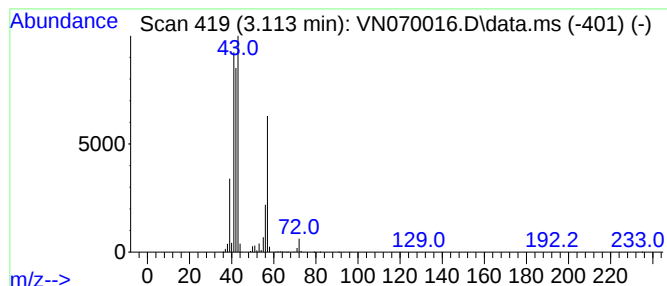
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.113	21.84 ug/l	2401320	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			Pentane	72	C5H12	000109-66-0	36
4			2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	25
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	14



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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A2-4-6.5

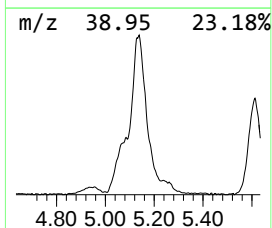
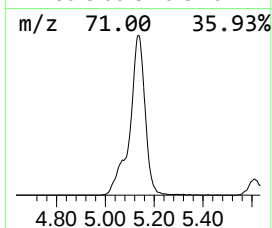
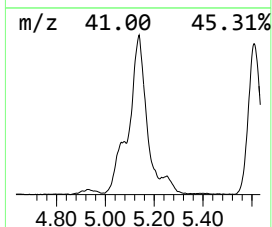
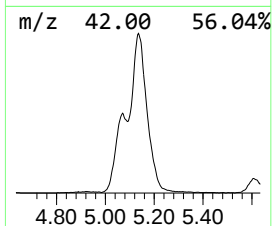
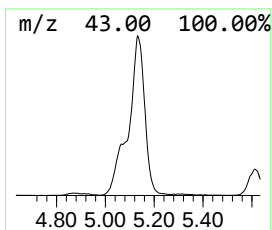
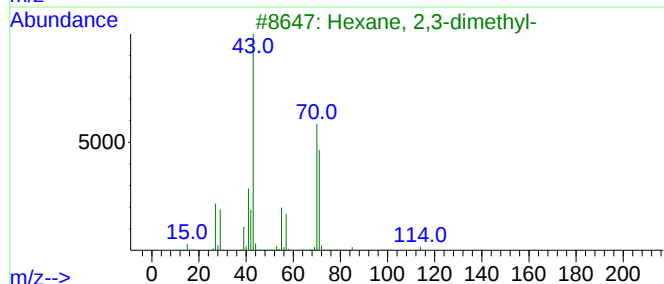
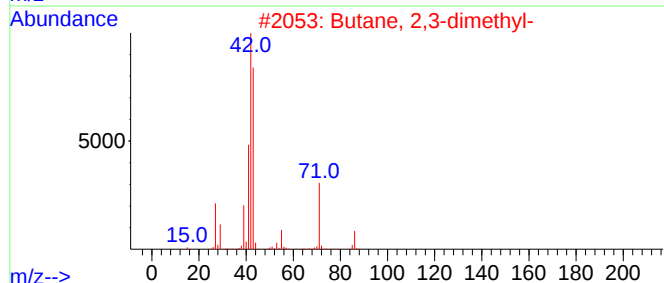
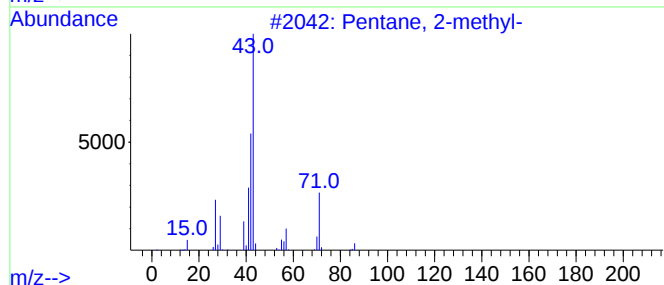
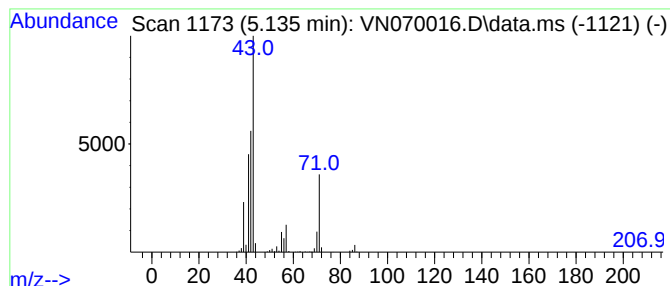
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.135	31.75 ug/l	3490700	Pentafluorobenzene	8.086

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	58
3			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	37
4			Pentane	72	C5H12	000109-66-0	37
5			Hexane, 3-ethyl-	114	C8H18	000619-99-8	37



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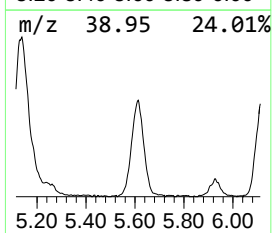
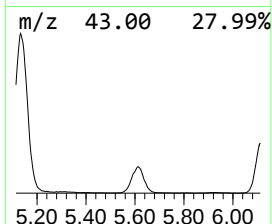
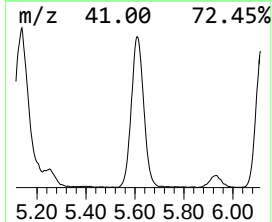
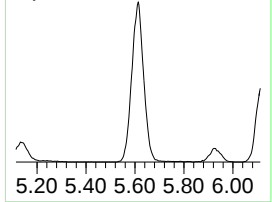
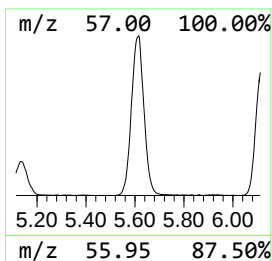
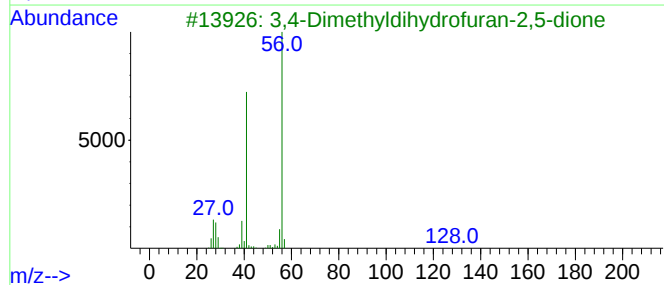
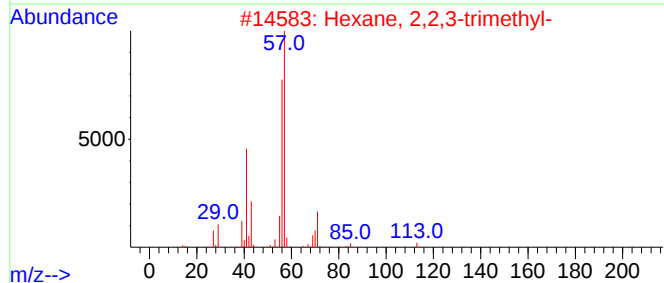
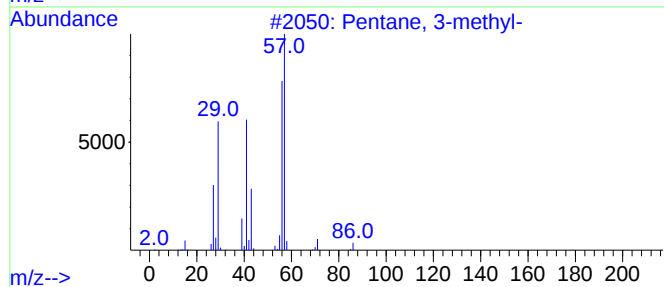
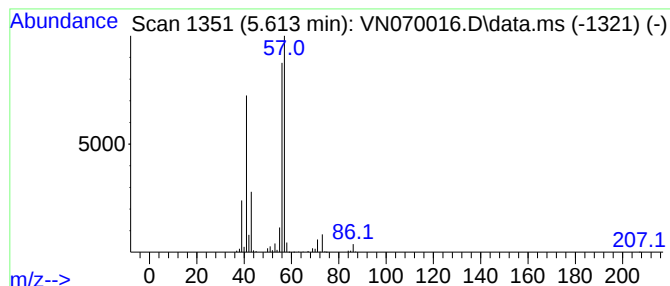
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.613	15.22 ug/l	1672860	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53
4			1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	40
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	40



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Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

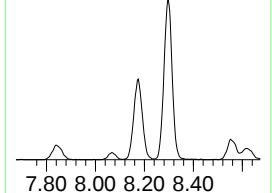
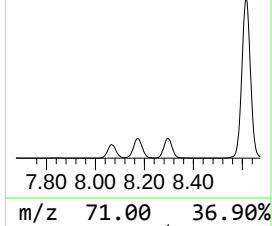
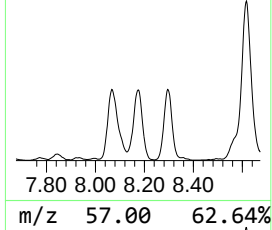
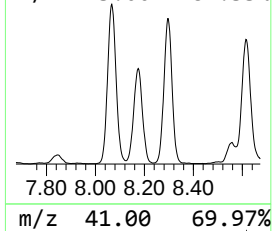
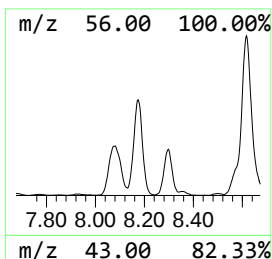
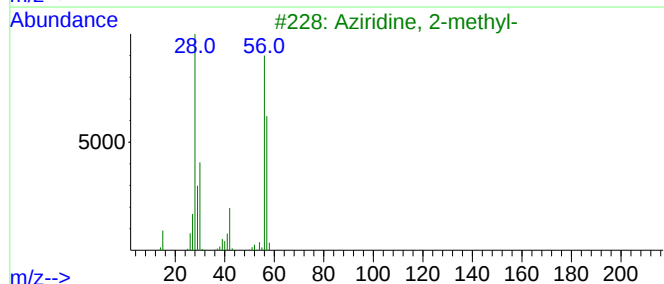
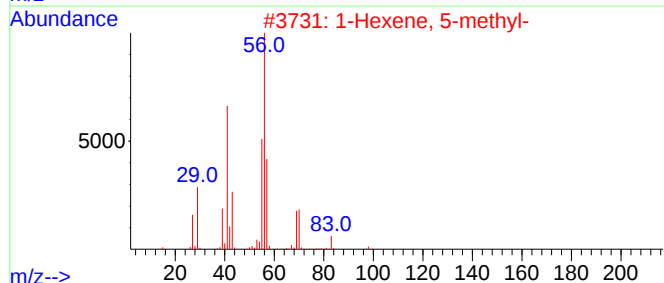
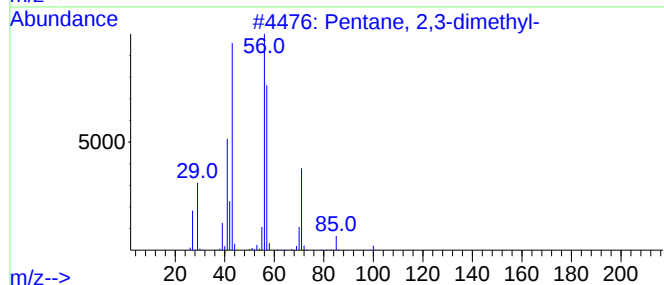
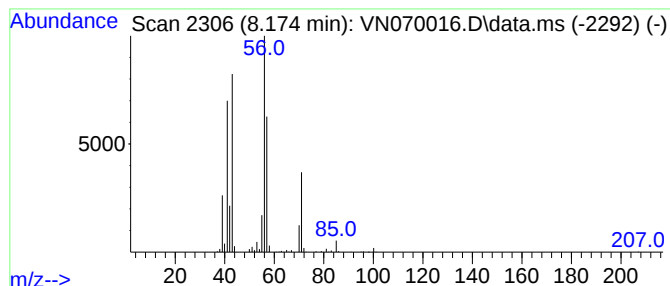
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Quant Title : SW846 8260

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

Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.174	16.07 ug/l	1767350	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			1-Hexene, 5-methyl-	98	C7H14	003524-73-0	50
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	47
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	47
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

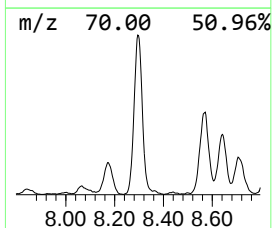
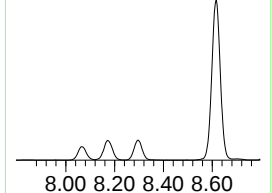
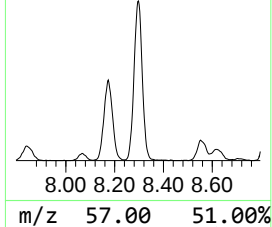
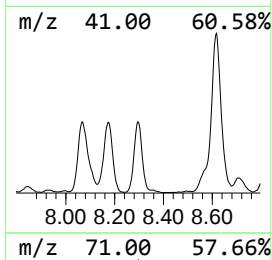
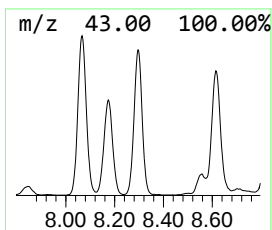
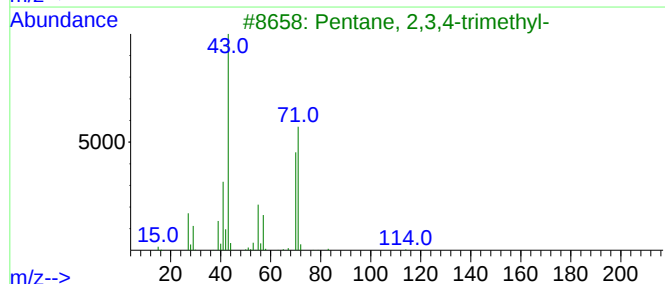
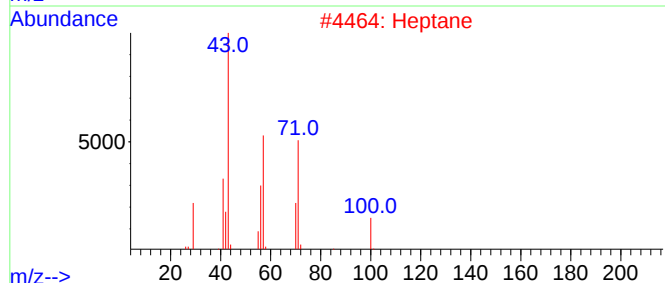
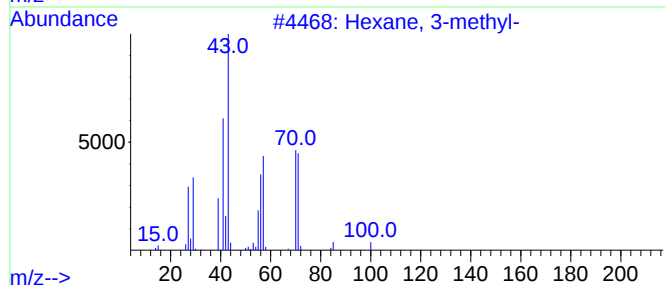
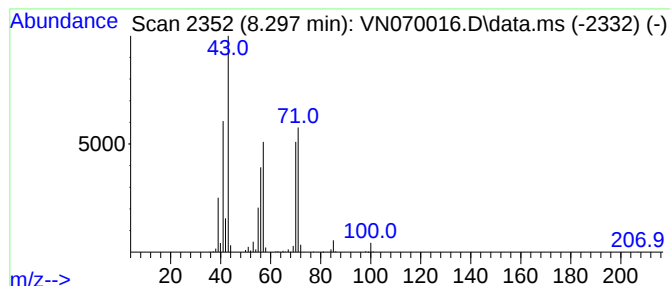
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.297	17.07 ug/l	1877130	Pentafluorobenzene	8.086

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	64
3			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	50
5			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

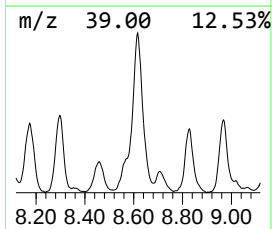
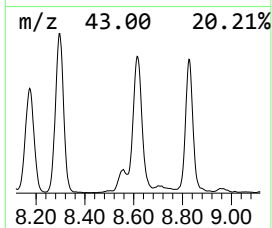
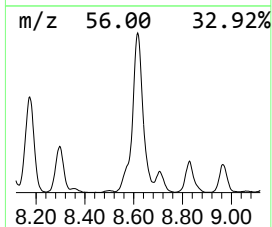
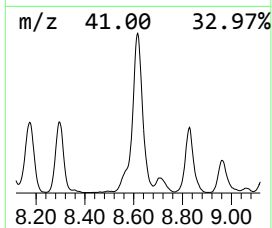
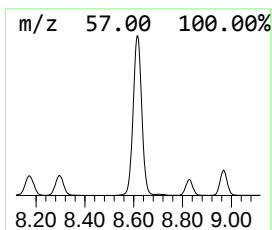
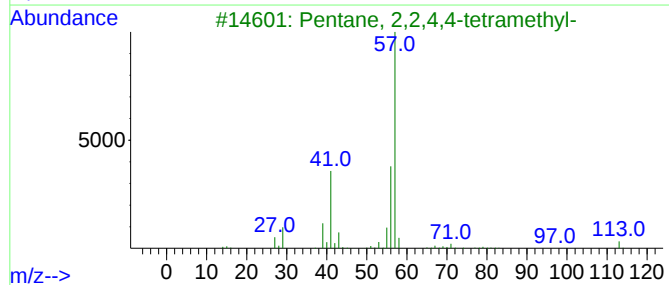
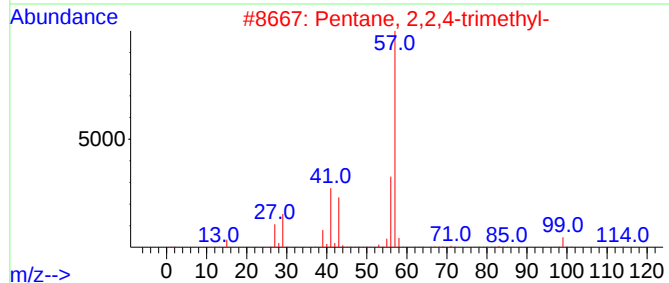
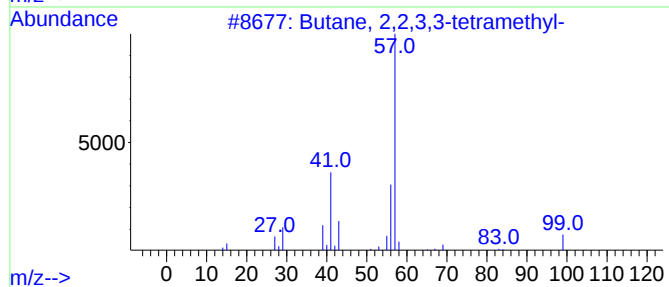
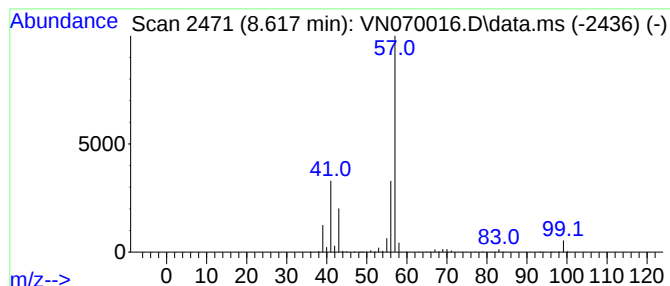
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Quant Title : SW846 8260

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

Peak Number 6 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.617	41.13 ug/l	5279800	1,4-Difluorobenzene	8.968

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

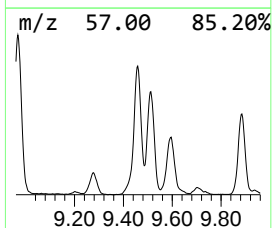
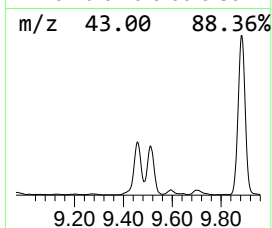
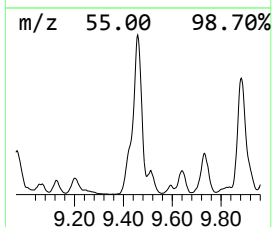
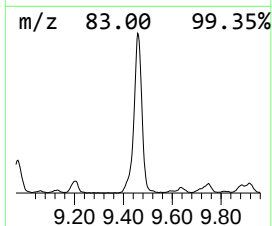
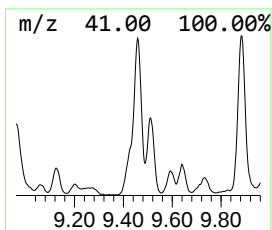
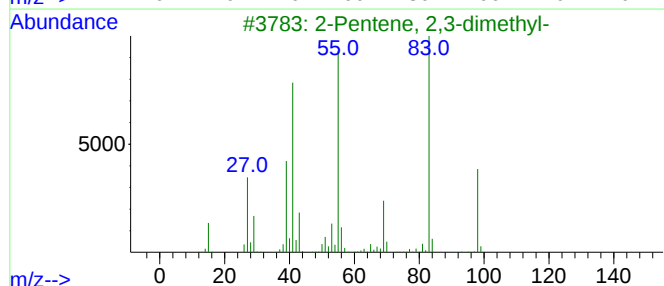
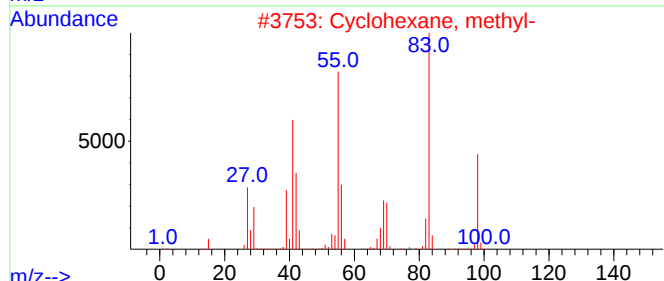
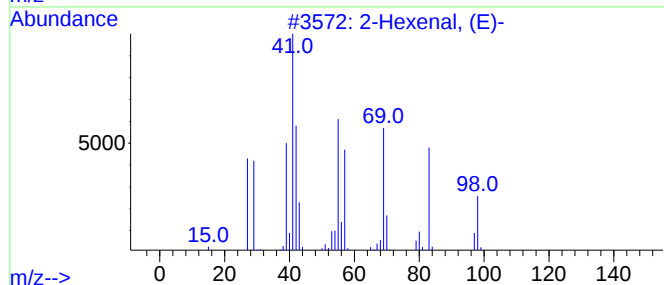
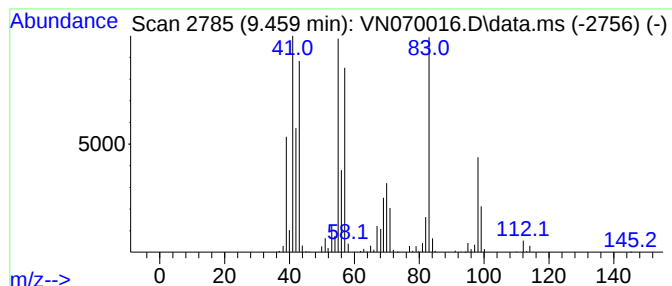
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Quant Title : SW846 8260

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

Peak Number 7 2-Hexenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.459	18.95 ug/l	2432290	1,4-Difluorobenzene	8.968

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hexenal, (E)-	98	C6H10O	006728-26-3	87
2		Cyclohexane, methyl-	98	C7H14	000108-87-2	64
3		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	60
4		2-Hexenal	98	C6H10O	000505-57-7	50
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

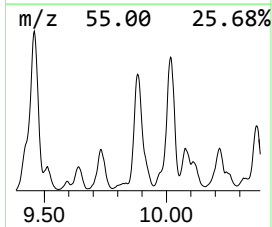
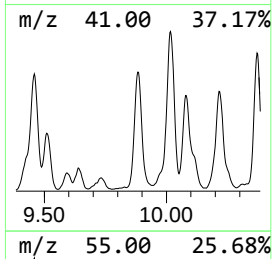
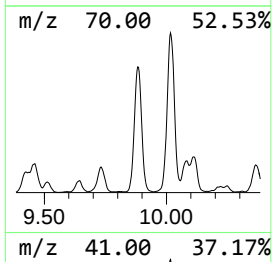
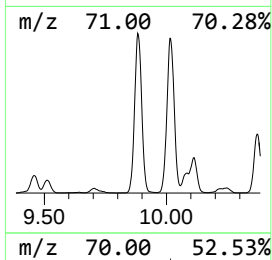
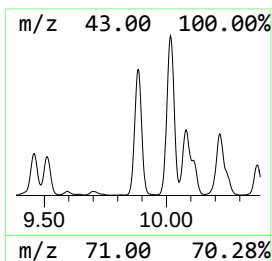
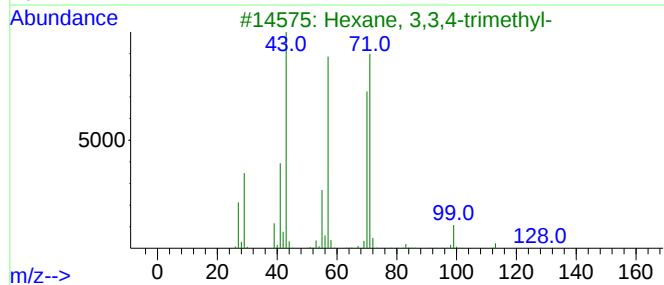
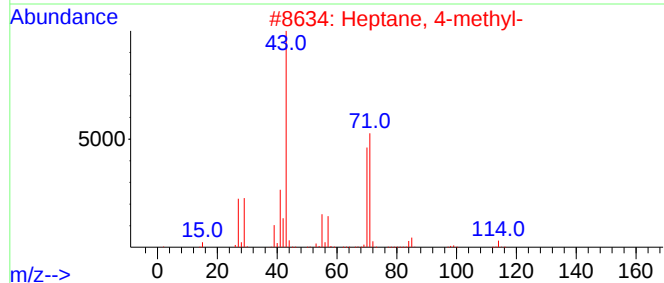
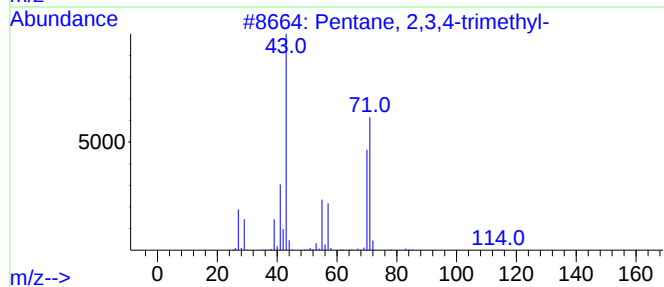
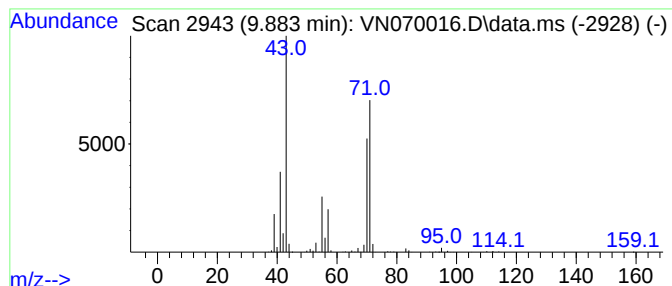
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.883	16.83 ug/l	2160410	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64
4			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	64
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

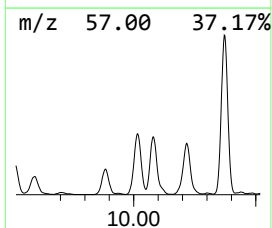
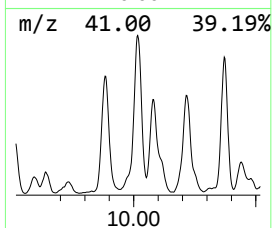
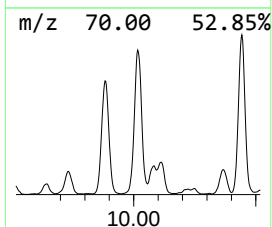
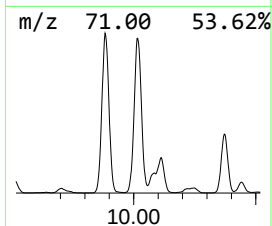
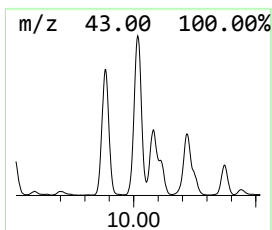
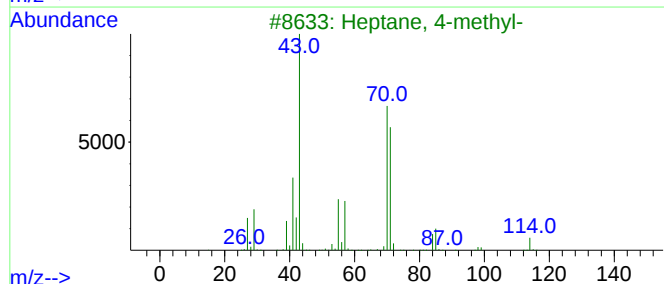
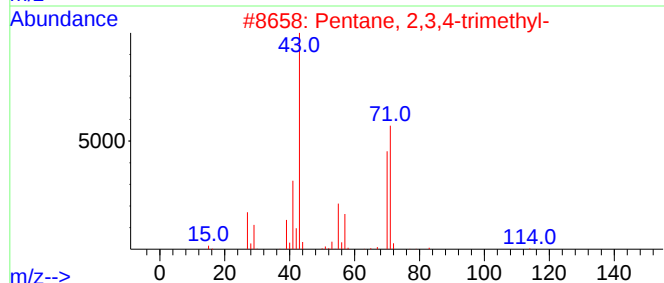
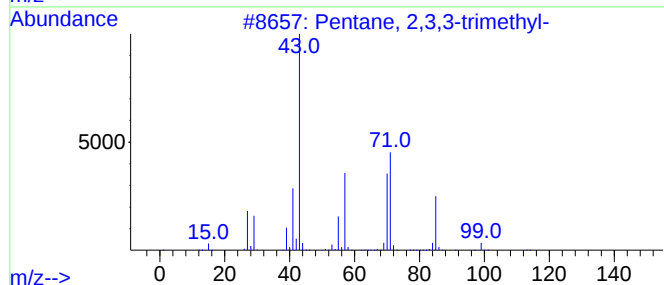
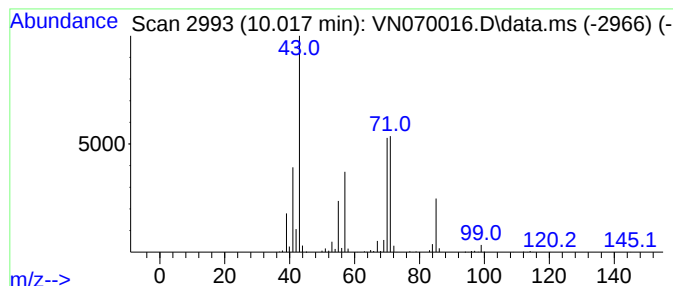
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.017	27.00 ug/l	3466520	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	74
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	72
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	59
5			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

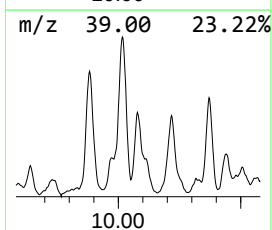
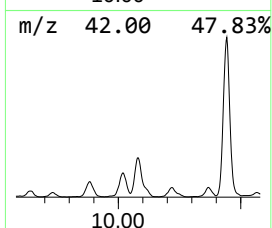
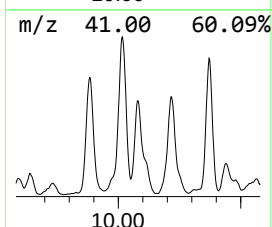
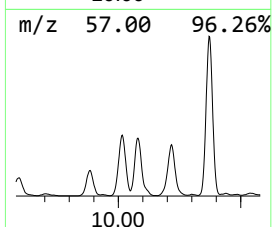
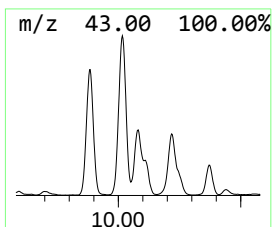
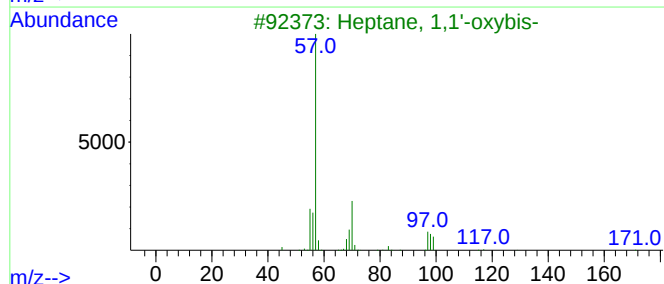
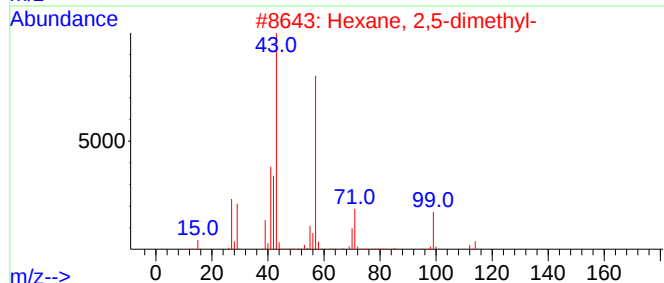
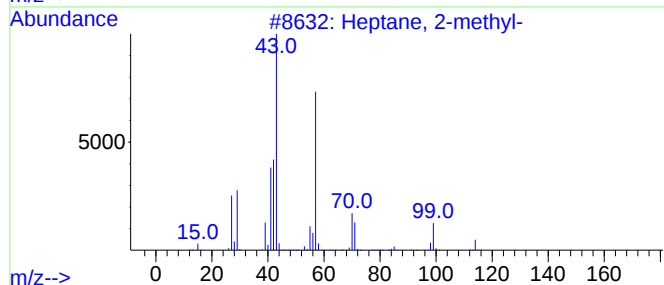
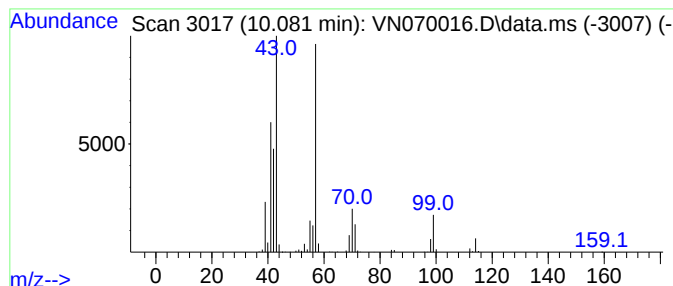
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Quant Title : SW846 8260

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

Peak Number 10 Heptane, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.081	13.82 ug/l	1774110	1,4-Difluorobenzene	8.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	91
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	72
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4			Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	50
5			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

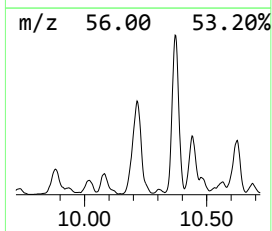
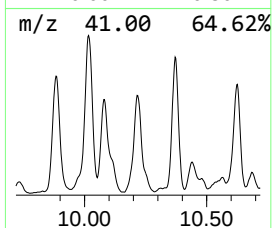
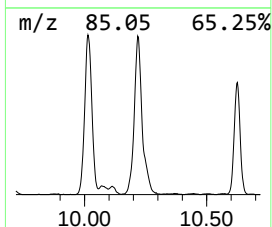
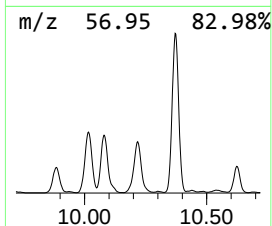
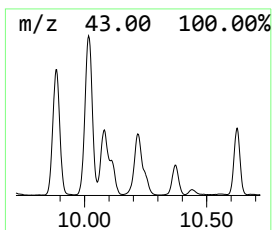
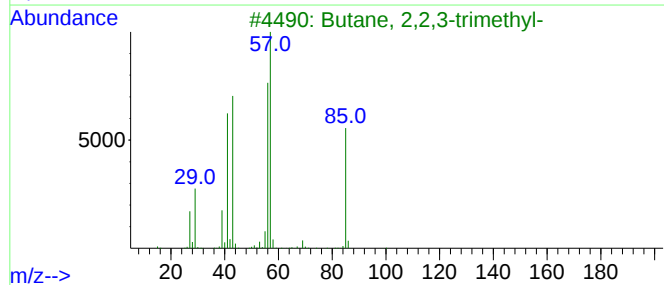
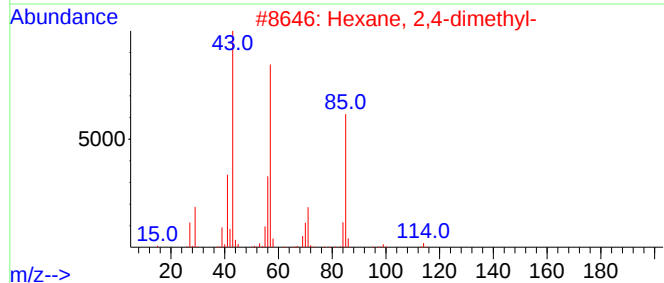
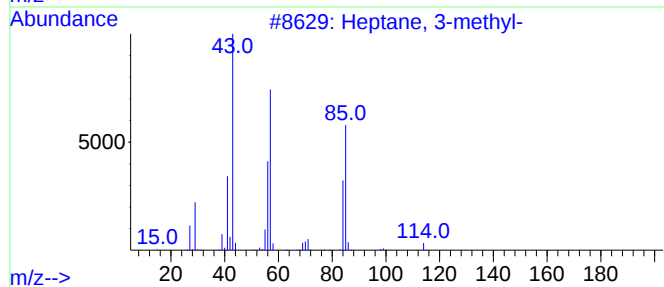
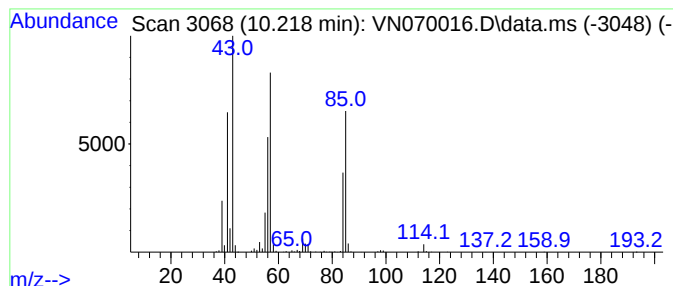
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Quant Title : SW846 8260

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

Peak Number 11 Heptane, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.218	13.03 ug/l	1672550	1,4-Difluorobenzene	8.968

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			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53
4			Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	53
5			Pentane, 3-ethyl-2,4-dimethyl-	128	C9H20	001068-87-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

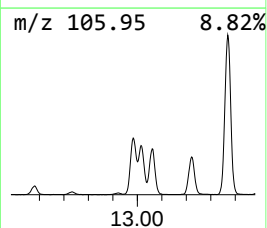
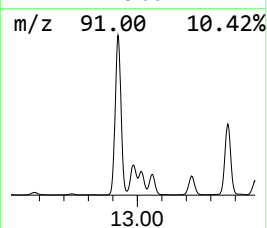
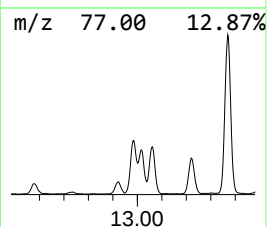
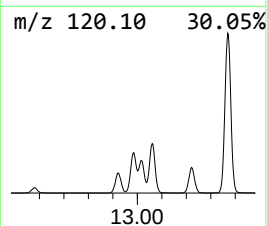
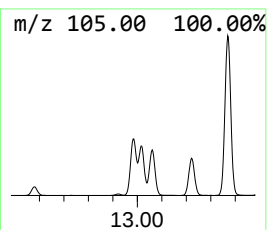
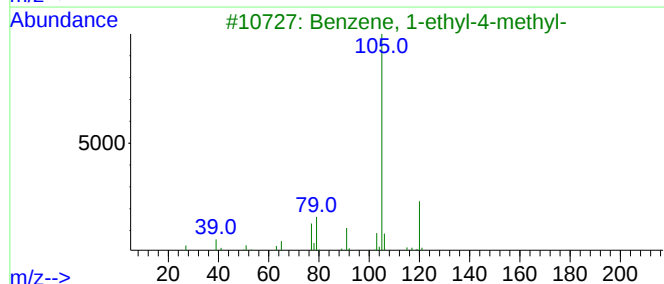
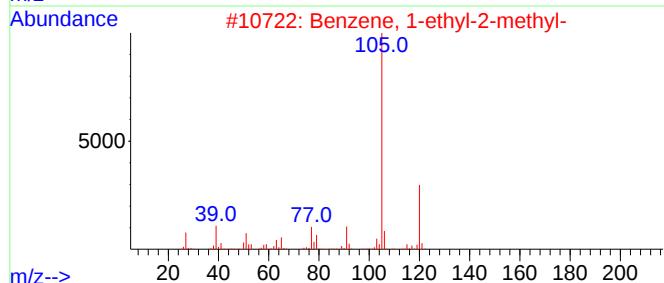
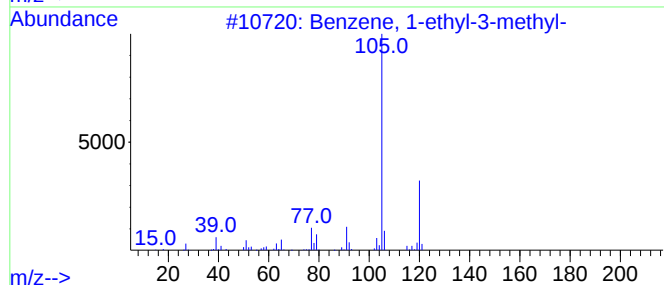
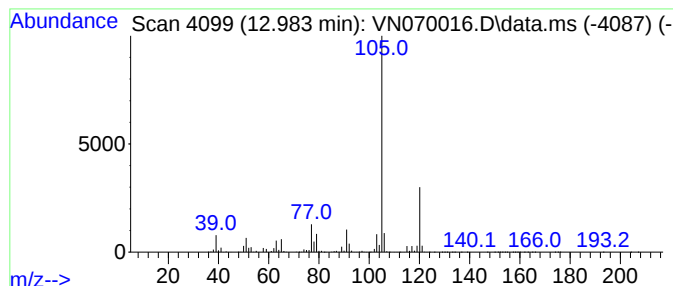
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Quant Title : SW846 8260

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

Peak Number 12 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.983	17.42 ug/l	4237500	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	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 : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

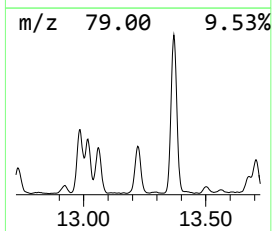
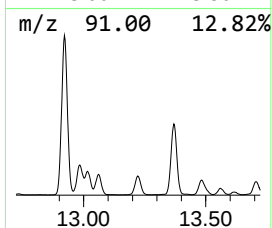
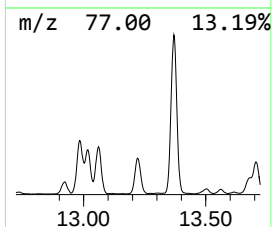
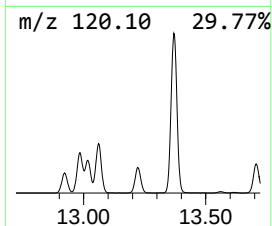
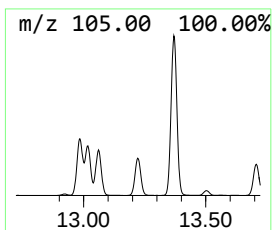
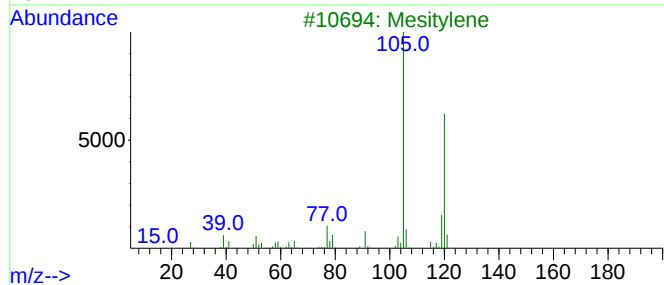
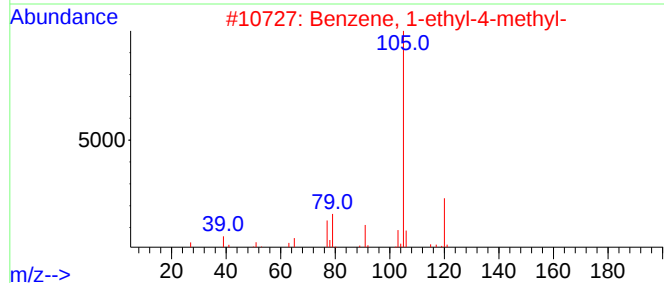
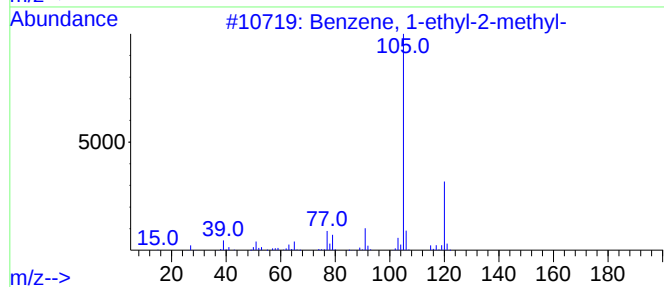
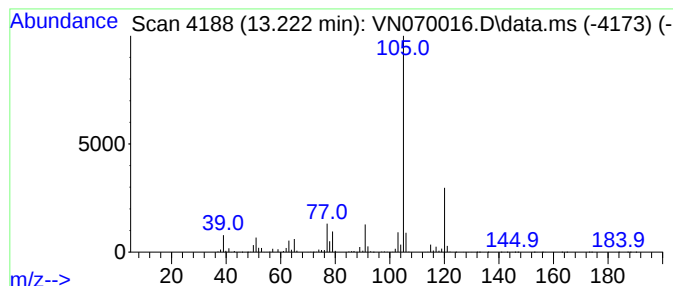
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Quant Title : SW846 8260

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

Peak Number 13 Benzene, 1-ethyl-2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.222	12.87 ug/l	3129870	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-4-methyl-	120	C9H12	000622-96-8	93
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

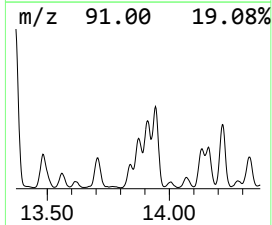
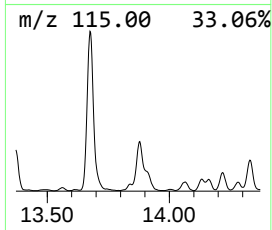
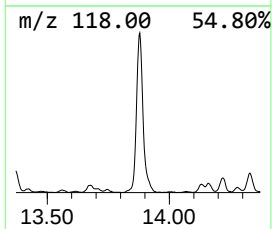
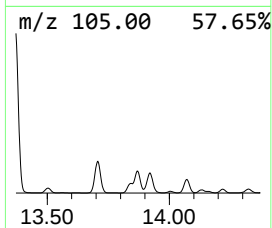
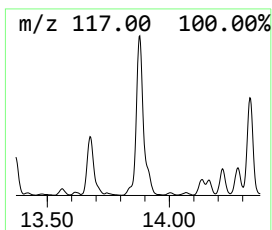
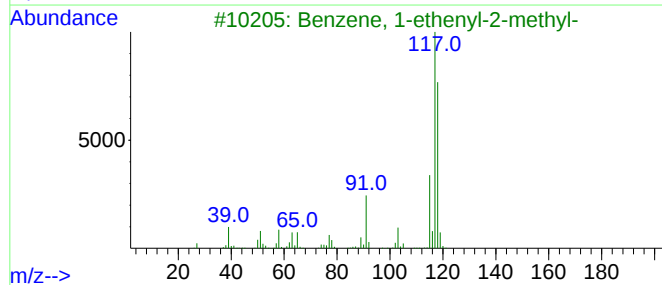
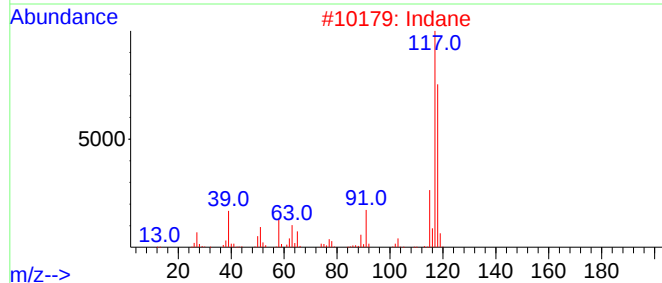
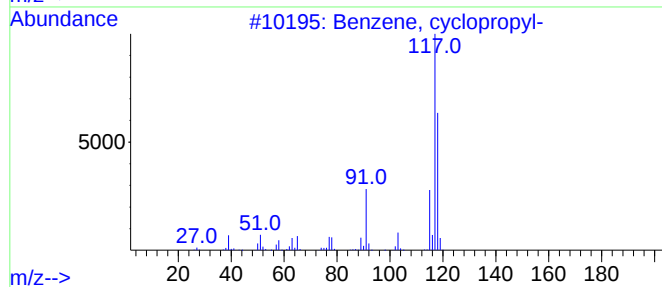
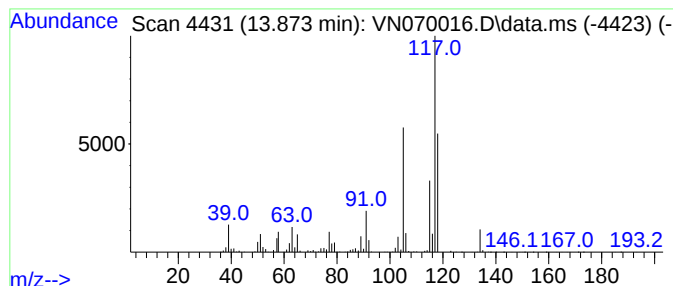
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Quant Title : SW846 8260

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

Peak Number 14 Benzene, cyclopropyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	13.62 ug/l	3313060	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
2			Indane	118	C9H10	000496-11-7	76
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	76
4			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	68
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

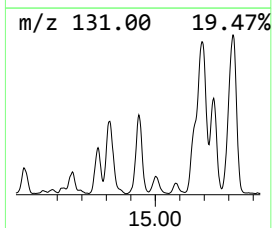
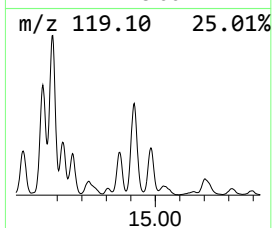
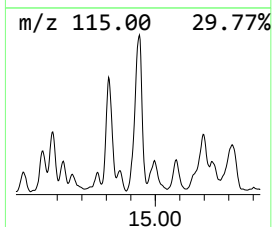
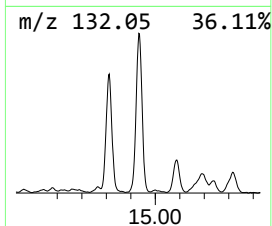
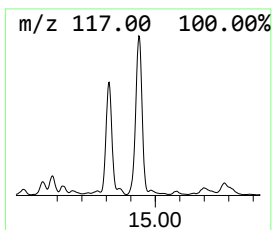
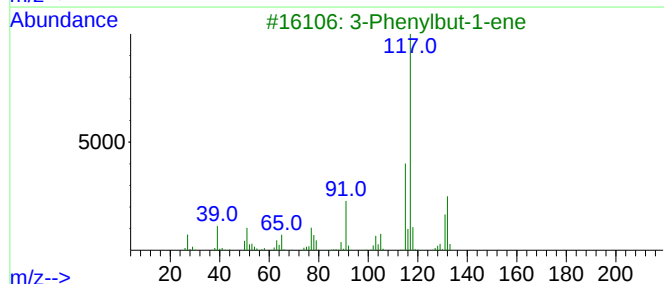
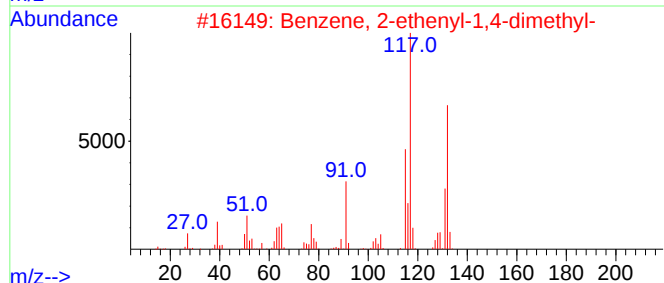
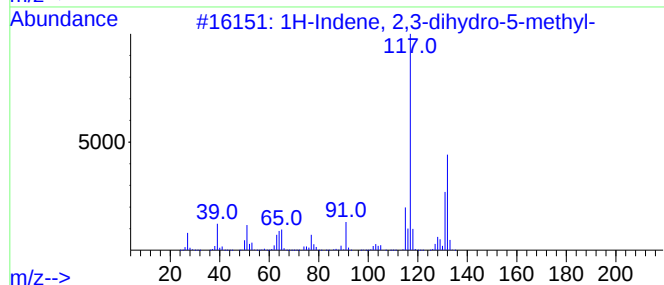
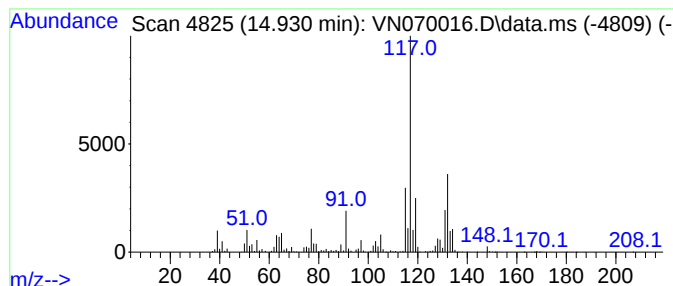
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Quant Title : SW846 8260

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

Peak Number 15 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	13.64 ug/l	3318690	1,4-Dichlorobenzene-d4	13.675

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	93
2			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	92
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
4			1-Phenyl-1-butene	132	C10H12	000824-90-8	81
5			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121121\
Data File : VN070016.D
Acq On : 11 Dec 2021 18:36
Operator : JC/MD
Sample : M4873-03 10X
Misc : 6.25g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
A2-4-6.5

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
Butane, 2-methyl-	3.113	21.8	ug/l	2401320	1	8.086	5497210	50.0
Pentane, 2-methyl-	5.135	31.8	ug/l	3490700	1	8.086	5497210	50.0
Pentane, 3-methyl-	5.613	15.2	ug/l	1672860	1	8.086	5497210	50.0
Pentane, 2,3-di...	8.174	16.1	ug/l	1767350	1	8.086	5497210	50.0
Hexane, 3-methyl-	8.297	17.1	ug/l	1877130	1	8.086	5497210	50.0
Butane, 2,2,3,3...	8.617	41.1	ug/l	5279800	2	8.968	6418830	50.0
2-Hexenal, (E)-	9.459	18.9	ug/l	2432290	2	8.968	6418830	50.0
Pentane, 2,3,4-...	9.883	16.8	ug/l	2160410	2	8.968	6418830	50.0
Pentane, 2,3,3-...	10.017	27.0	ug/l	3466520	2	8.968	6418830	50.0
Heptane, 2-methyl-	10.081	13.8	ug/l	1774110	2	8.968	6418830	50.0
Heptane, 3-methyl-	10.218	13.0	ug/l	1672550	2	8.968	6418830	50.0
Benzene, 1-ethy...	12.983	17.4	ug/l	4237500	4	13.675	12162200	50.0
Benzene, 1-ethy...	13.222	12.9	ug/l	3129870	4	13.675	12162200	50.0
Benzene, cyclop...	13.873	13.6	ug/l	3313060	4	13.675	12162200	50.0
1H-Indene, 2,3-...	14.930	13.6	ug/l	3318690	4	13.675	12162200	50.0