

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
 Data File : VN070243.D
 Acq On : 20 Dec 2021 16:19
 Operator : JC/MD
 Sample : M5044-13
 Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-13-4.5

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: VN070243.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.003	368	378	402	rVB3	327393	704976	4.11%	0.311%
2	3.411	512	530	556	rVB3	220918	554380	3.23%	0.245%
3	4.189	792	820	851	rBV3	108860	377579	2.20%	0.167%
4	5.033	1105	1135	1140	rBV3	254308	741271	4.32%	0.327%
5	5.581	1306	1339	1374	rBV	361598	1262088	7.36%	0.557%
6	6.087	1499	1528	1562	rBV4	315423	990874	5.78%	0.437%
7	6.444	1646	1661	1686	rVB4	71394	219850	1.28%	0.097%
8	6.879	1798	1823	1848	rBV4	83844	269715	1.57%	0.119%
9	7.026	1851	1878	1898	rBV2	581329	1775815	10.35%	0.784%
10	7.128	1899	1916	1937	rVB2	261886	735361	4.29%	0.324%
11	7.831	2164	2178	2197	rVB4	101124	255610	1.49%	0.113%
12	8.021	2224	2249	2253	rBV2	950432	2040859	11.90%	0.901%
13	8.163	2288	2302	2327	rVB	1211168	3019787	17.60%	1.332%
14	8.284	2328	2347	2369	rBV	1118303	2615754	15.25%	1.154%
15	8.431	2382	2402	2431	rBV	1117362	2666977	15.55%	1.177%
16	8.606	2432	2467	2492	rBV	5266135	13718493	79.97%	6.053%
17	8.818	2525	2546	2577	rVB	799031	1771142	10.33%	0.782%
18	8.963	2577	2600	2627	rBV	3089200	6981434	40.70%	3.080%
19	9.118	2646	2658	2672	rVB4	106111	206950	1.21%	0.091%
20	9.451	2749	2782	2793	rBV2	1808395	4145845	24.17%	1.829%
21	9.504	2793	2802	2818	rVB	1209650	2350419	13.70%	1.037%
22	9.587	2819	2833	2844	rBV	358401	729326	4.25%	0.322%
23	9.727	2864	2885	2901	rVB5	155075	450266	2.62%	0.199%
24	9.877	2924	2941	2964	rBV	3593191	7327806	42.72%	3.233%
25	10.011	2965	2991	3005	rBV	4839168	10411120	60.69%	4.594%
26	10.076	3005	3015	3024	rBV	882776	1484954	8.66%	0.655%
27	10.212	3045	3066	3092	rBV2	1283499	3171650	18.49%	1.399%
28	10.365	3110	3123	3137	rVV	2610544	4780406	27.87%	2.109%
29	10.440	3137	3151	3173	rVB	4735663	9183466	53.54%	4.052%
30	10.620	3203	3218	3232	rVB2	1009524	1960673	11.43%	0.865%
31	10.682	3233	3241	3251	rVB4	147300	215943	1.26%	0.095%
32	10.805	3268	3287	3296	rVB6	176945	461497	2.69%	0.204%
33	10.885	3297	3317	3334	rVV7	631396	1740263	10.15%	0.768%
34	10.961	3335	3345	3358	rVB2	284356	507165	2.96%	0.224%
35	11.049	3359	3378	3391	rBV3	301647	629471	3.67%	0.278%
36	11.151	3406	3416	3433	rVB	485845	988375	5.76%	0.436%

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37	11.454	3520	3529	3537	rBV2	265173	416793	2.43%	0.184%
38	11.524	3540	3555	3581	rVB3	1229933	2882916	16.81%	1.272%
39	11.626	3581	3593	3615	rBV	990868	1776736	10.36%	0.784%
40	11.744	3617	3637	3653	rBV	5294185	10292676	60.00%	4.542%
41	11.813	3656	3663	3664	rVV2	486200	552132	3.22%	0.244%
42	11.843	3665	3674	3694	rVB	2182262	3836689	22.37%	1.693%
43	11.958	3702	3717	3740	rVB	3061995	6312698	36.80%	2.785%
44	12.184	3793	3801	3813	rVB5	260190	407990	2.38%	0.180%
45	12.253	3818	3827	3830	rBV5	267935	359968	2.10%	0.159%
46	12.363	3860	3868	3879	rVB2	322456	530028	3.09%	0.234%
47	12.580	3938	3949	3958	rBV	787188	1381610	8.05%	0.610%
48	12.731	3990	4005	4027	rVB2	4422784	10463446	61.00%	4.617%
49	12.873	4048	4058	4065	rBV2	449340	815459	4.75%	0.360%
50	12.918	4066	4075	4092	rVB	1978239	3276196	19.10%	1.446%
51	13.015	4099	4111	4119	rBV	2823585	4798930	27.98%	2.117%
52	13.219	4173	4187	4204	rBV	2013676	3814112	22.24%	1.683%
53	13.313	4215	4222	4229	rVB	609612	773966	4.51%	0.342%
54	13.366	4230	4242	4255	rVB	10776122	17153520	100.00%	7.569%
55	13.530	4297	4303	4323	rVB2	985542	1861029	10.85%	0.821%
56	13.605	4324	4331	4337	rBV5	335879	480636	2.80%	0.212%
57	13.672	4345	4356	4364	rBV	5275640	9206784	53.67%	4.062%
58	13.836	4407	4417	4423	rBV	1116333	1720911	10.03%	0.759%
59	13.876	4424	4432	4440	rVV3	1402044	2221688	12.95%	0.980%
60	13.994	4468	4476	4491	rVB3	658777	960106	5.60%	0.424%
61	14.066	4494	4503	4515	rVB	1057675	1702550	9.93%	0.751%
62	14.131	4515	4527	4532	rBV	1911454	3104400	18.10%	1.370%
63	14.214	4547	4558	4574	rVB	3333386	5389810	31.42%	2.378%
64	14.324	4589	4599	4612	rVB3	1244947	2128685	12.41%	0.939%
65	14.458	4640	4649	4661	rVB	683060	1046758	6.10%	0.462%
66	14.538	4668	4679	4686	rBV	1927767	3176607	18.52%	1.402%
67	14.576	4686	4693	4703	rVV	2905371	4407198	25.69%	1.945%
68	14.621	4703	4710	4731	rVB4	1184065	2122258	12.37%	0.936%
69	14.761	4755	4762	4769	rBV2	281784	370988	2.16%	0.164%
70	14.809	4769	4780	4788	rVV3	1500860	2647202	15.43%	1.168%
71	14.847	4790	4794	4806	rVB4	1105266	1478294	8.62%	0.652%
72	14.922	4806	4822	4836	rBV5	2261529	5890971	34.34%	2.599%
73	14.978	4838	4843	4859	rVB	647392	1100761	6.42%	0.486%
74	15.195	4913	4924	4950	rVB4	1184577	3006108	17.52%	1.326%
75	15.305	4955	4965	4984	rVB4	755415	1594582	9.30%	0.704%
76	15.504	5027	5039	5054	rVB	1842732	3535989	20.61%	1.560%

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77	15.611	5069	5079	5090	rBV3	353052	628921	3.67%	0.278%
78	15.804	5137	5151	5172	rBV	578483	1289957	7.52%	0.569%
79	16.107	5256	5264	5276	rVB	261555	450160	2.62%	0.199%
80	16.614	5438	5453	5492	rVB	1613672	3816646	22.25%	1.684%

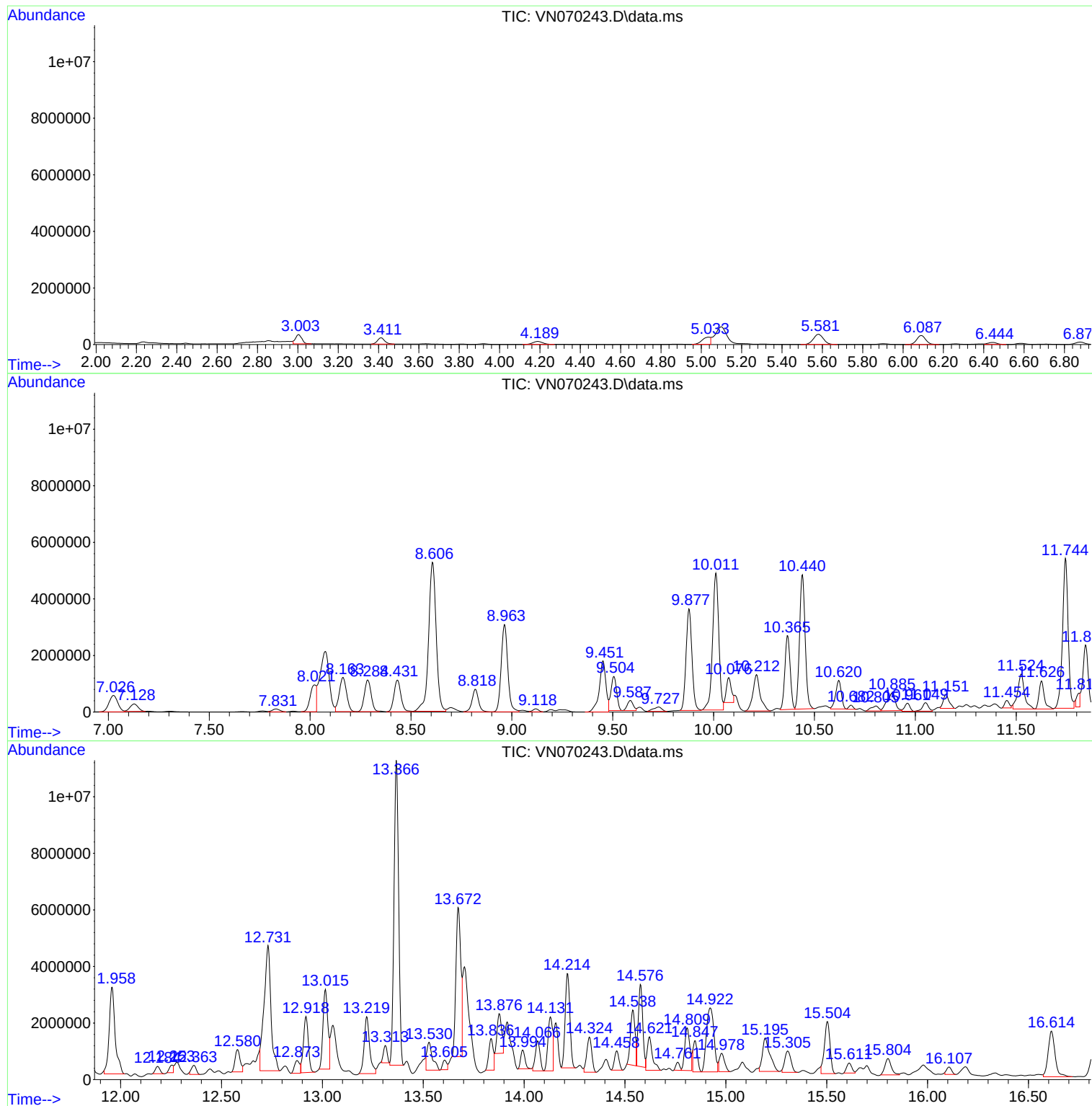
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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



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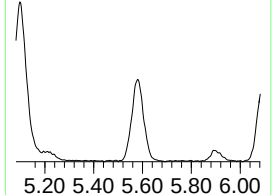
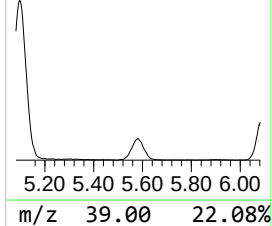
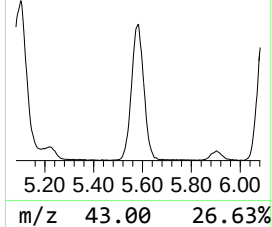
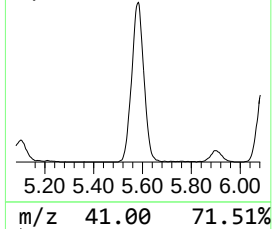
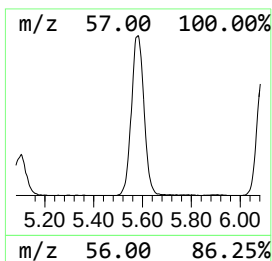
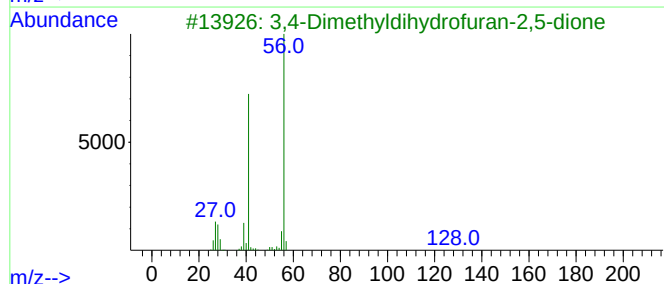
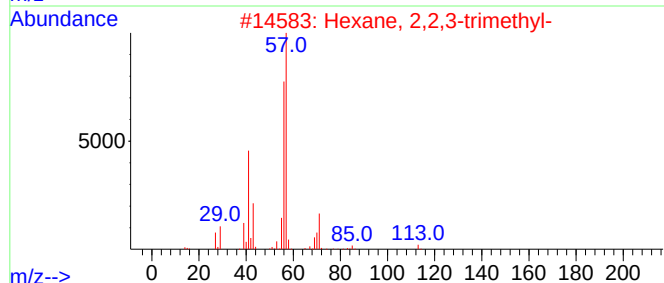
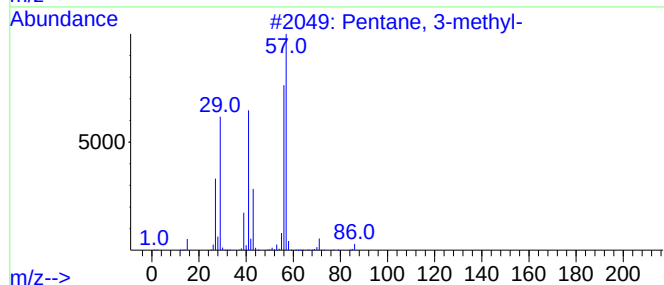
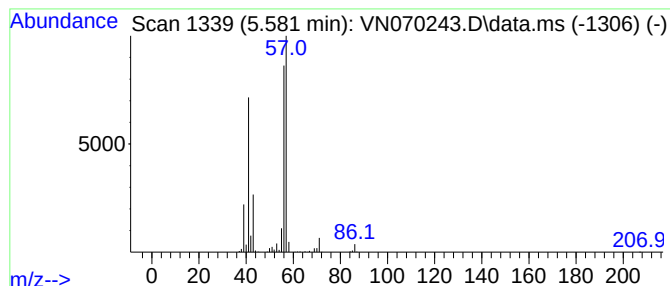
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N120221W.M
Quant Title : SW846 8260

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

Peak Number 1 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.581	30.92 ug/l	1262090	Pentafluorobenzene	8.080

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	64
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	53
4			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5			Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40



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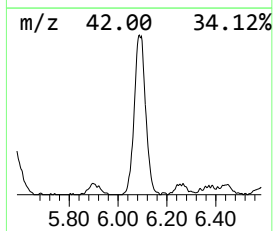
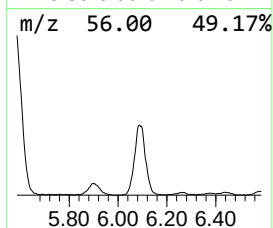
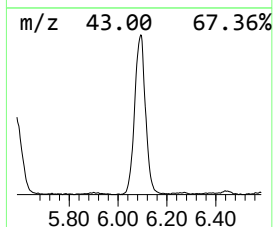
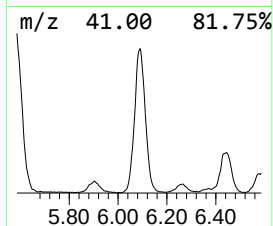
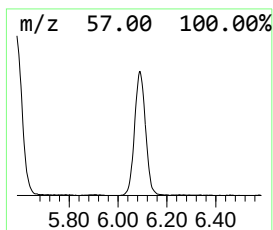
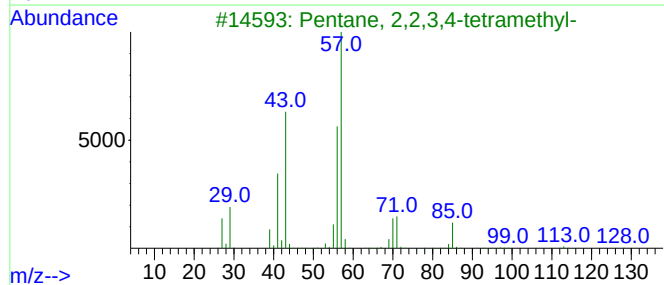
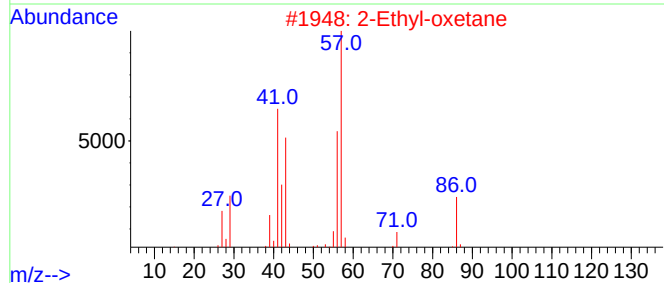
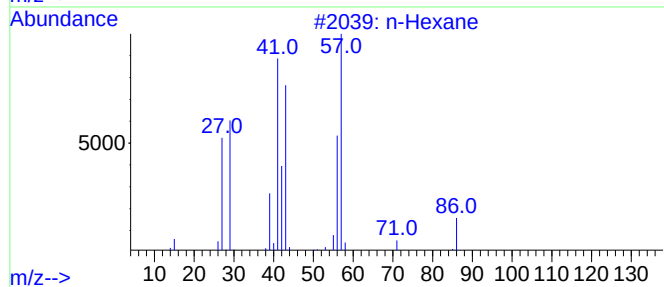
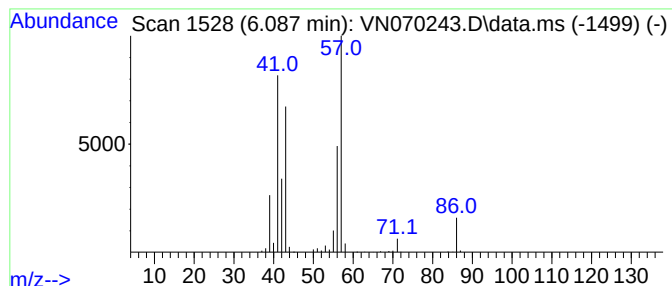
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.087	24.28 ug/l	990874	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	78
3	Pentane, 2,2,3,4-tetramethyl-		128	C9H20	001186-53-4	38
4	1-Pentene, 4-methyl-		84	C6H12	000691-37-2	38
5	Propanal, 2,2-dimethyl-		86	C5H10O	000630-19-3	35



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Instrument :
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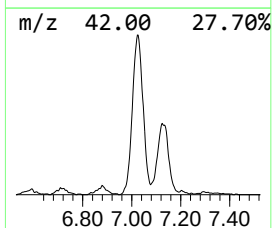
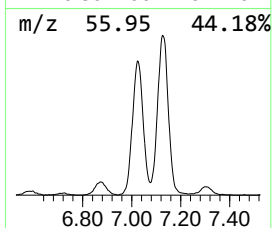
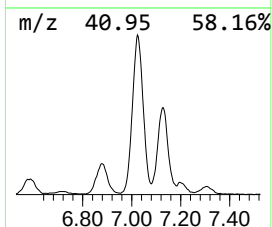
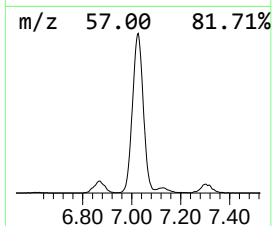
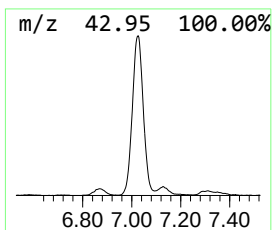
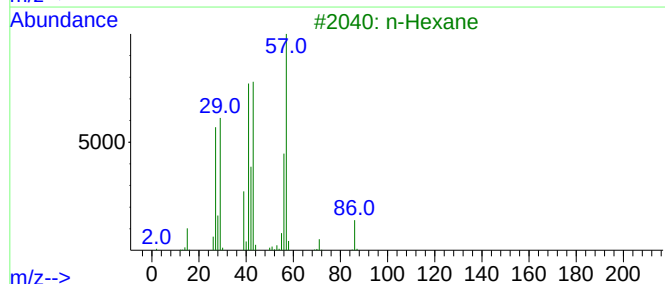
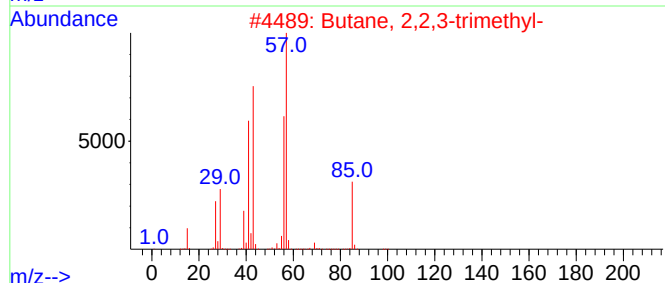
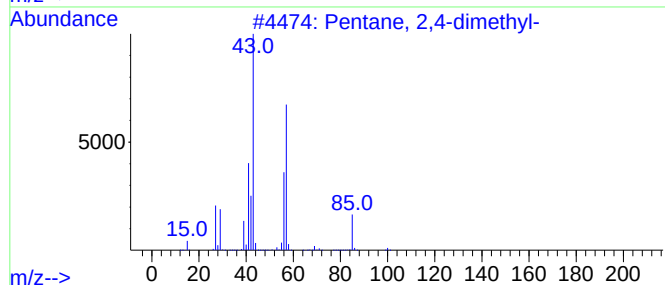
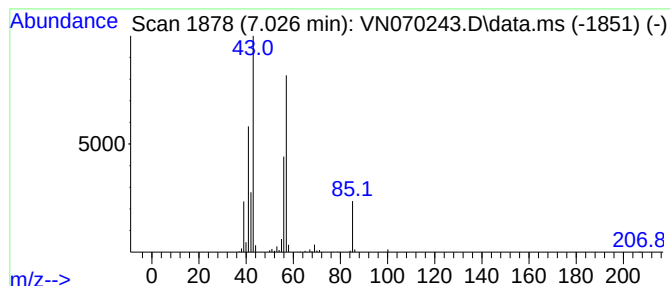
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.026	43.51 ug/l	1775820	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3			n-Hexane	86	C6H14	000110-54-3	53
4			2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	50
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50



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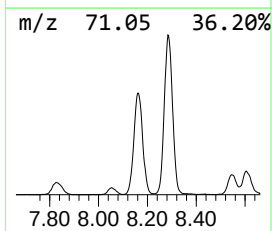
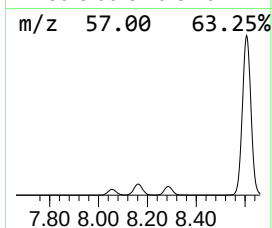
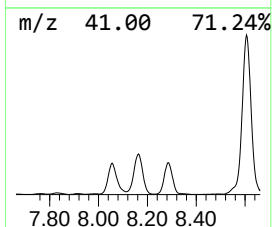
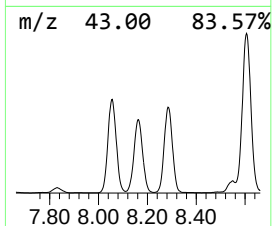
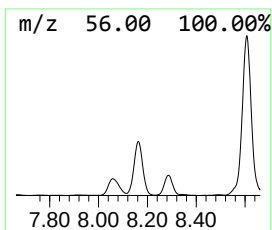
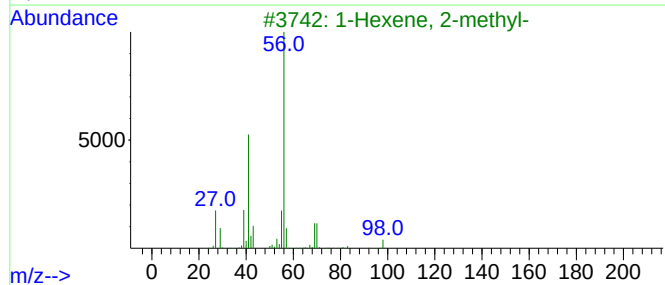
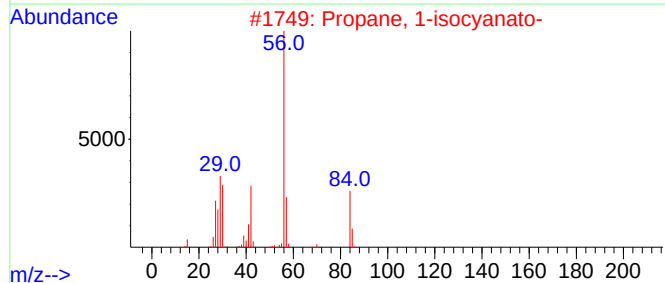
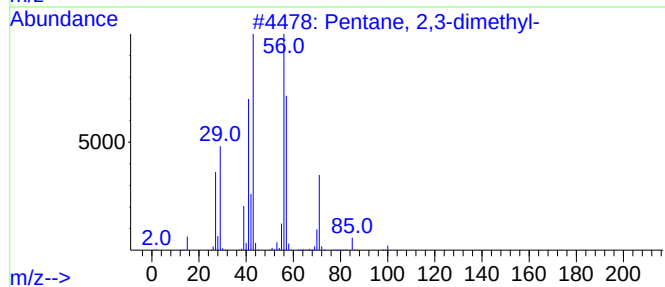
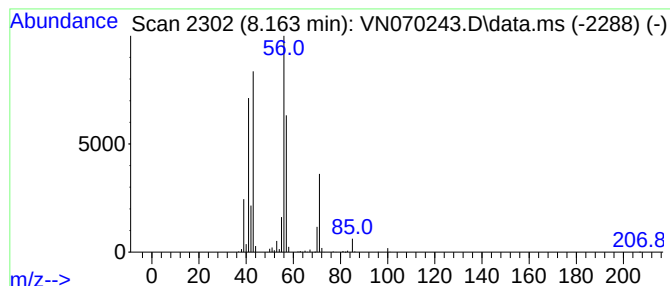
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.163	73.98 ug/l	3019790	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	50
3			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	47
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	33
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

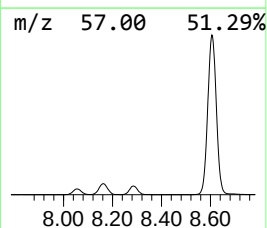
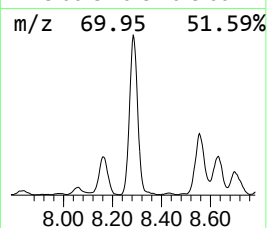
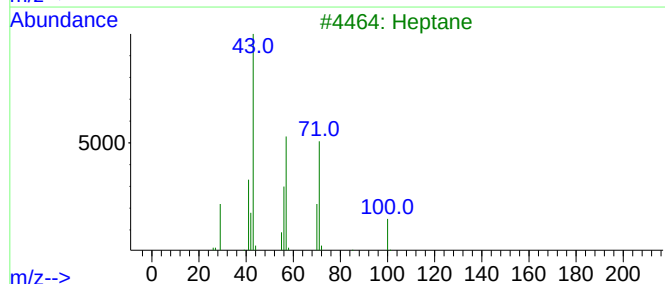
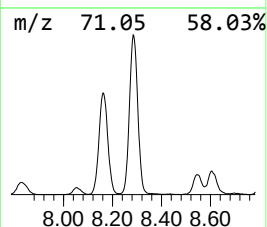
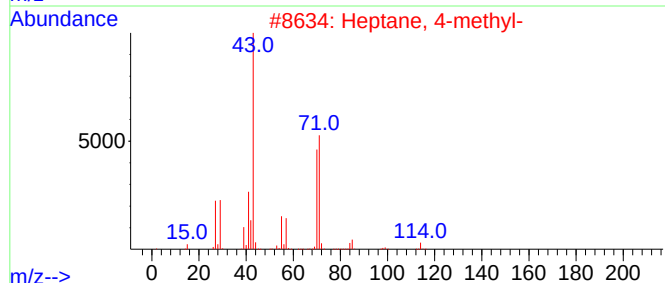
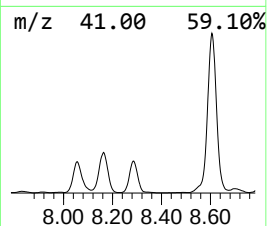
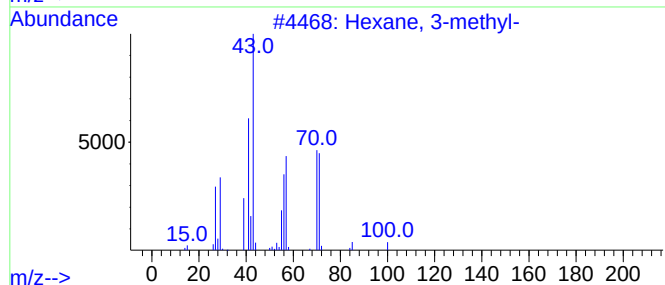
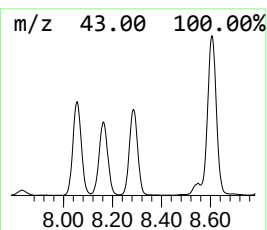
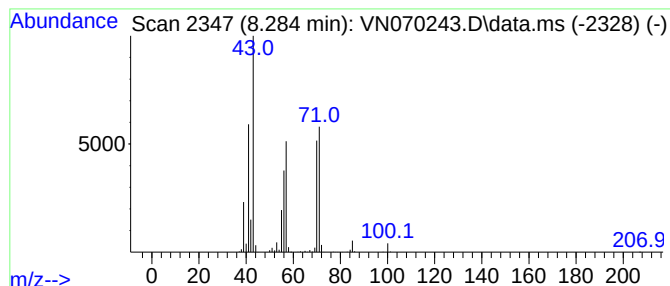
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Quant Title : SW846 8260

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

Peak Number 5 Hexane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.284	64.08 ug/l	2615750	Pentafluorobenzene	8.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3-methyl-	100	C7H16	000589-34-4	95
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3			Heptane	100	C7H16	000142-82-5	64
4			Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5			Pentane, 3-ethyl-	100	C7H16	000617-78-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

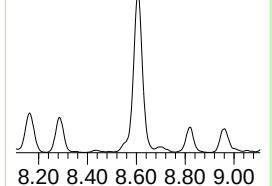
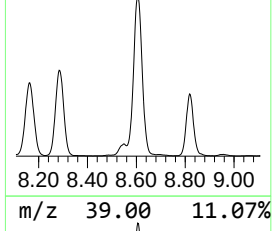
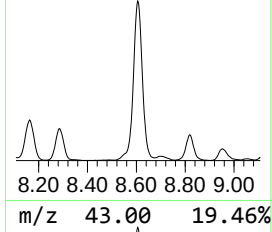
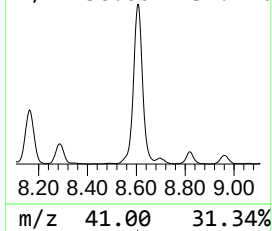
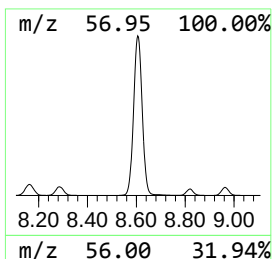
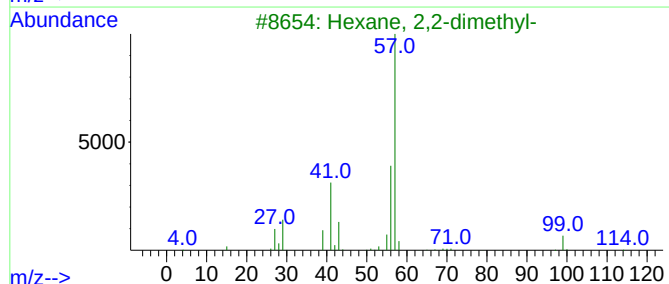
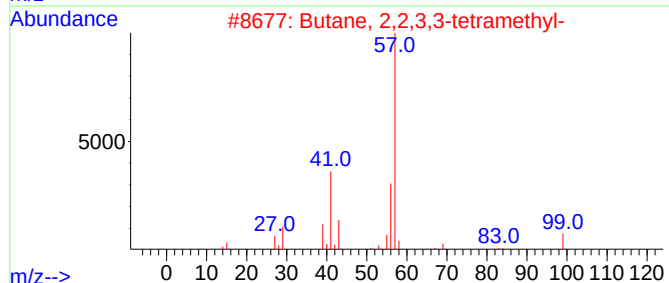
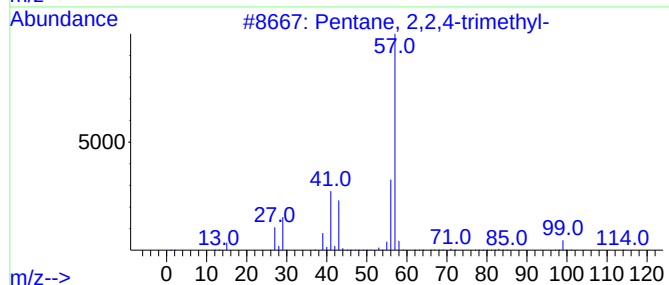
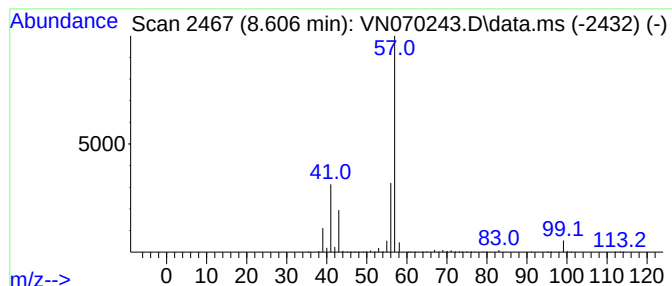
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.606	98.25 ug/l	13718500	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	83
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

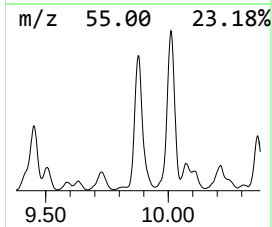
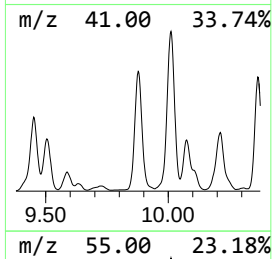
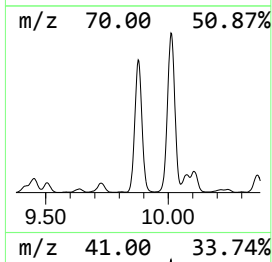
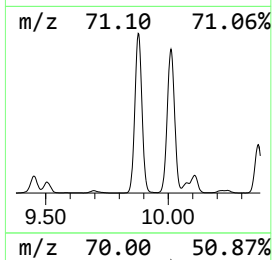
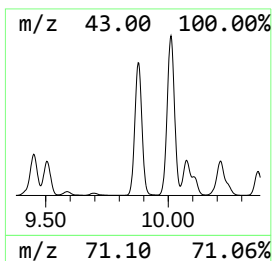
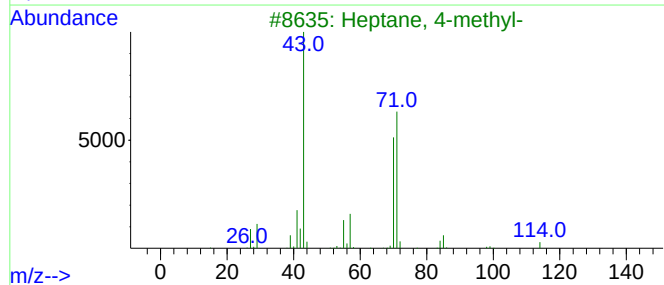
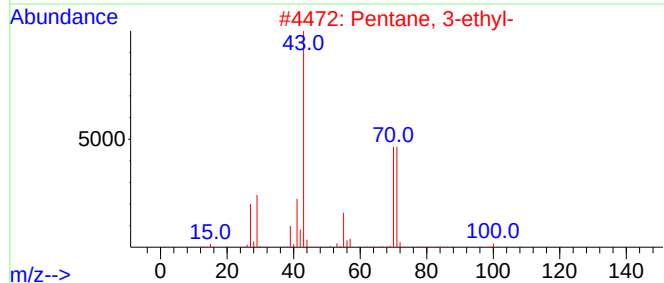
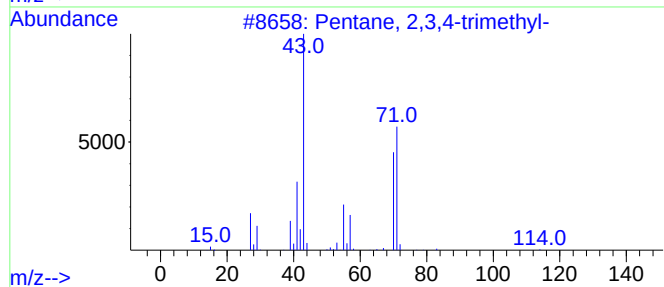
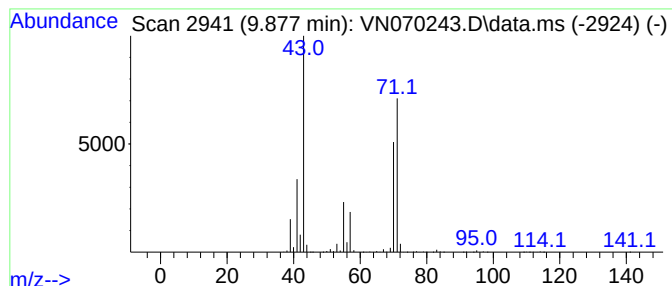
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.877	52.48 ug/l	7327810	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	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	72
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

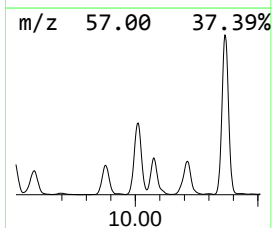
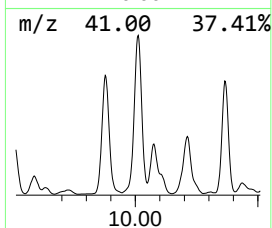
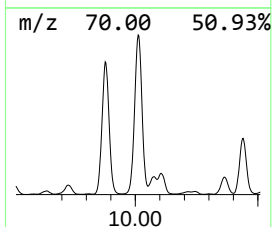
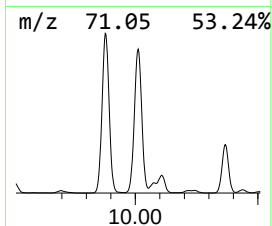
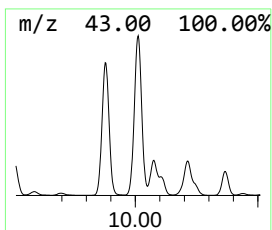
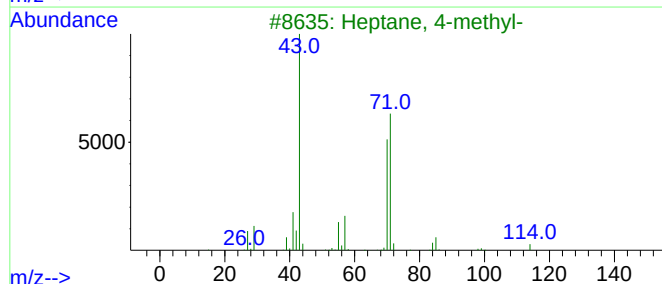
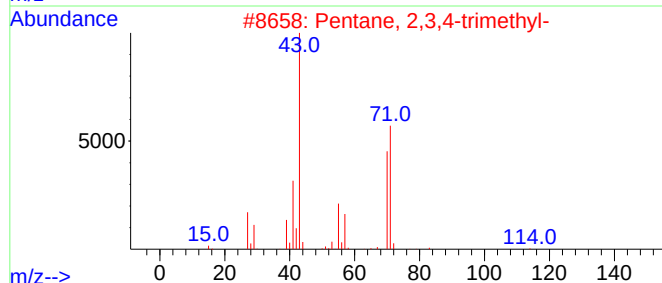
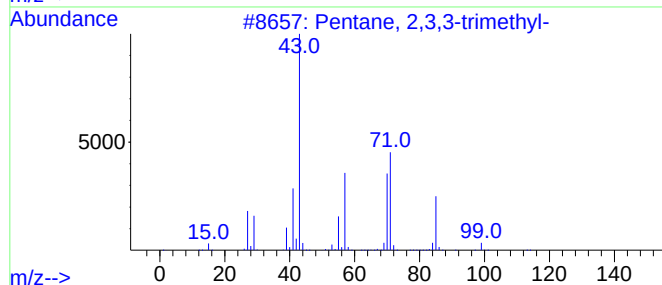
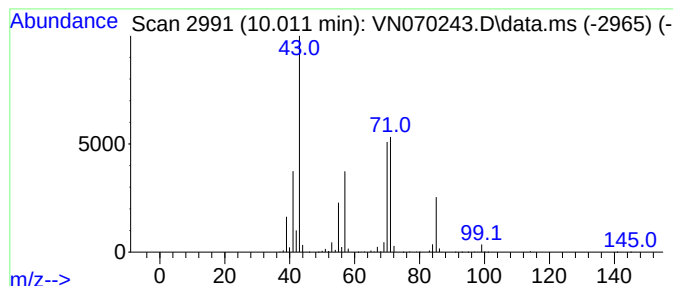
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.011	74.56 ug/l	10411100	1,4-Difluorobenzene	8.965

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	76
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

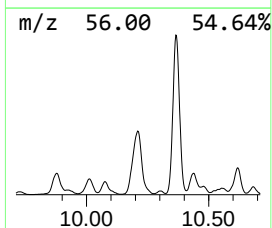
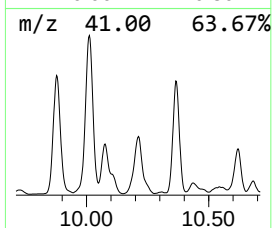
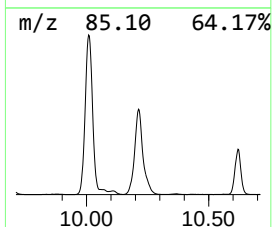
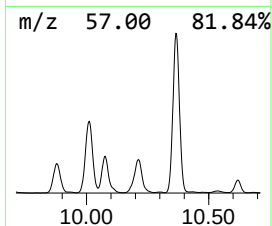
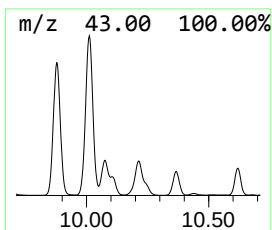
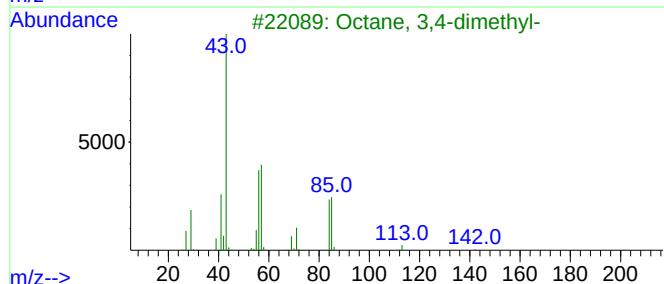
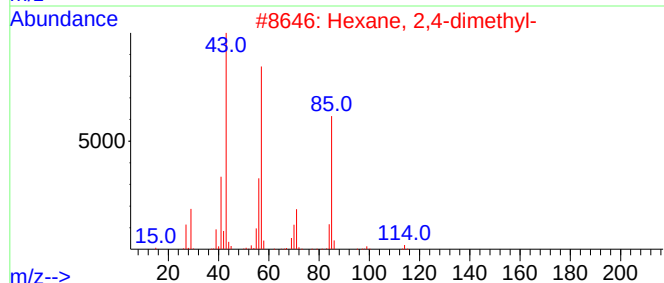
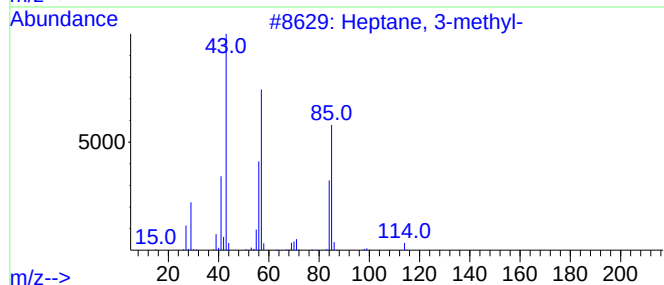
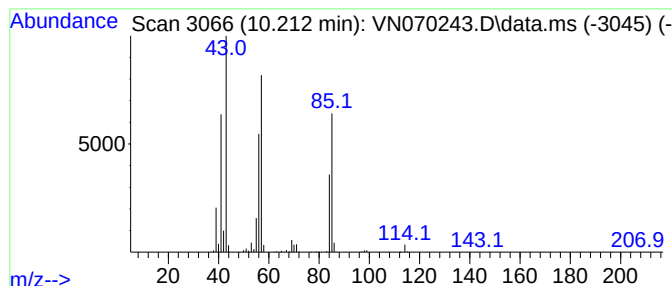
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Quant Title : SW846 8260

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.
10.212	22.71 ug/l	3171650	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			Octane, 3,4-dimethyl-	142	C10H22	015869-92-8	53
4			Pentanoic acid, butyl ester	158	C9H18O2	000591-68-4	50
5			Pentane, 2,3,3,4-tetramethyl-	128	C9H20	016747-38-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

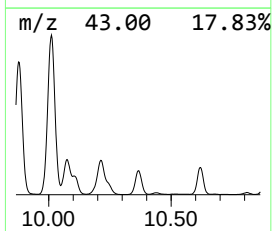
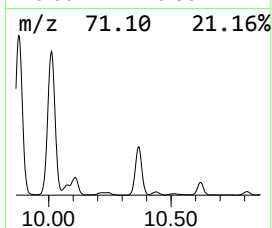
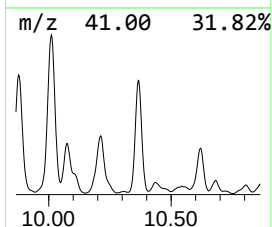
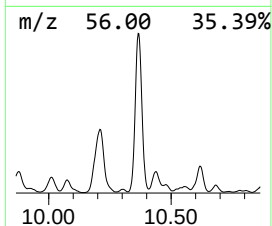
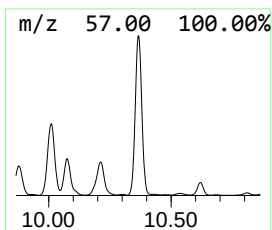
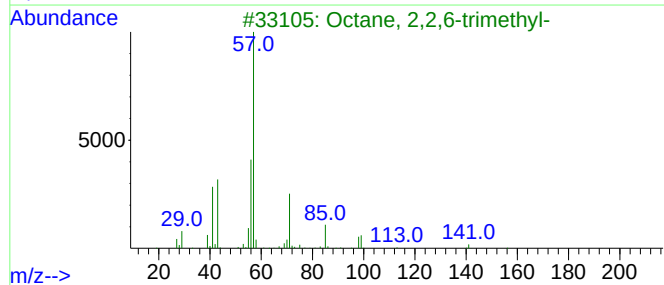
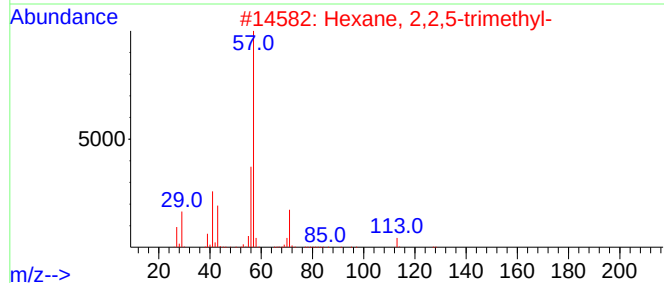
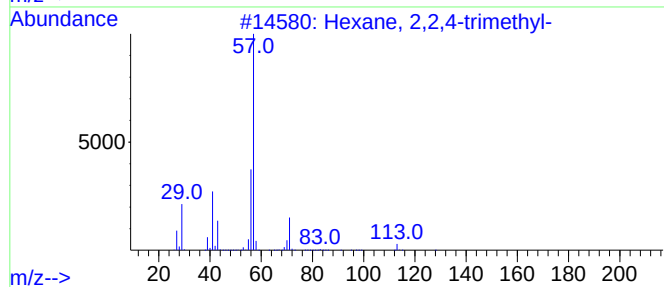
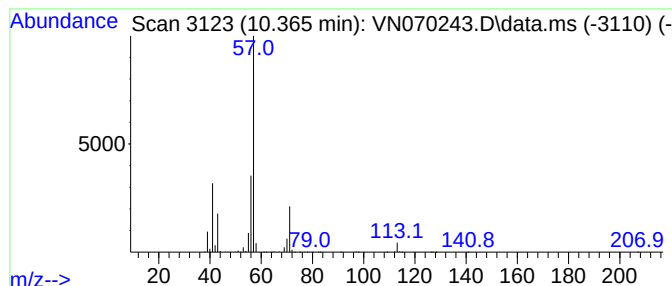
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Quant Title : SW846 8260

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

Peak Number 10 Hexane, 2,2,4-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	23.22 ug/l	4780410	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	83
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	83
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

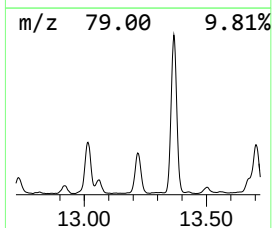
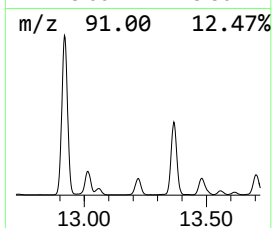
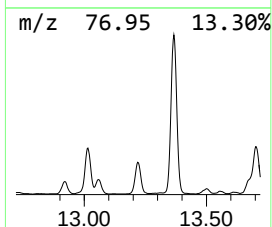
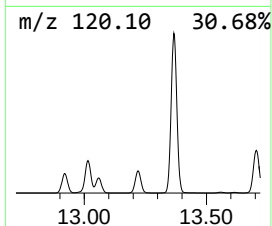
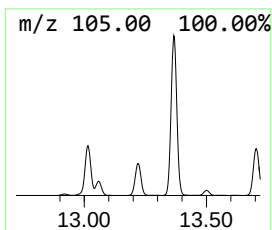
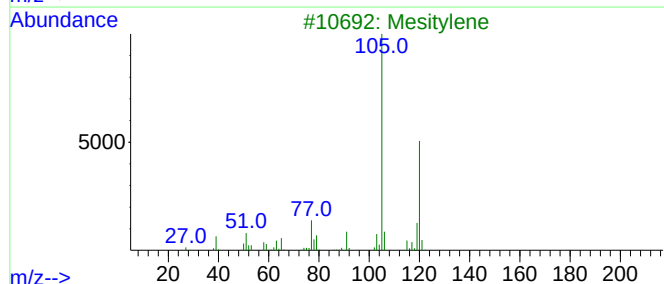
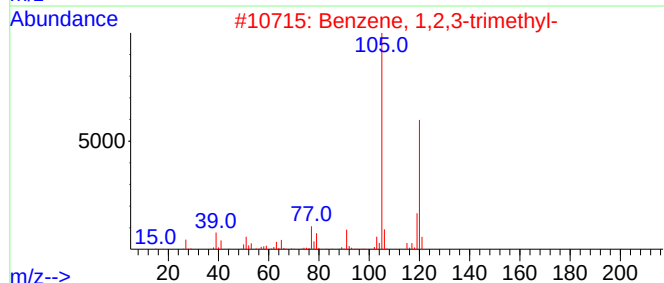
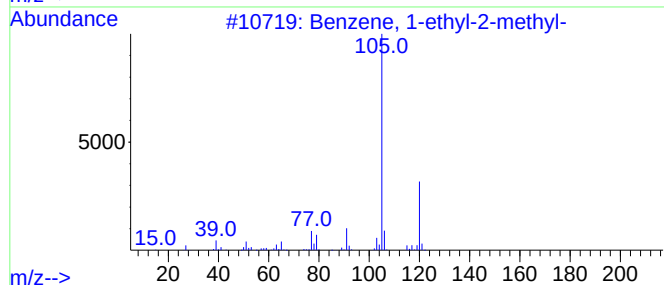
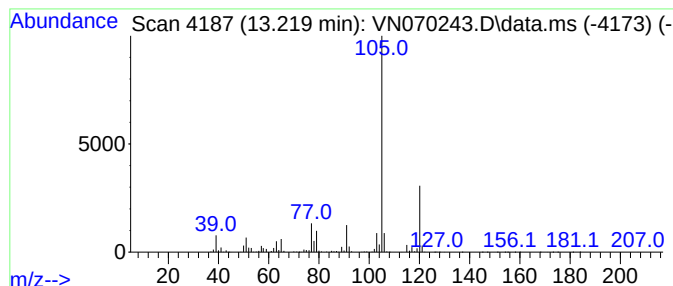
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Quant Title : SW846 8260

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

Peak Number 11 Benzene, 1-ethyl-2-methyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	20.71 ug/l	3814110	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

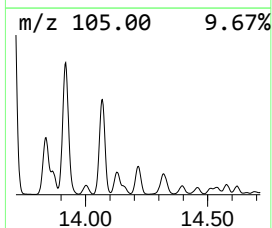
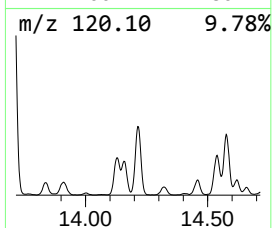
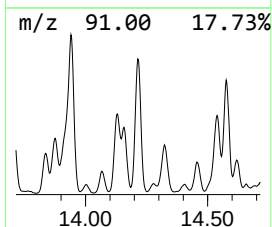
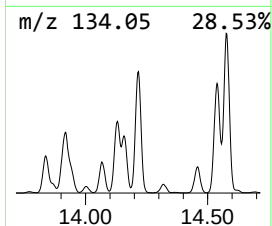
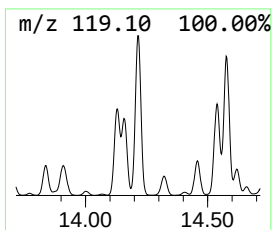
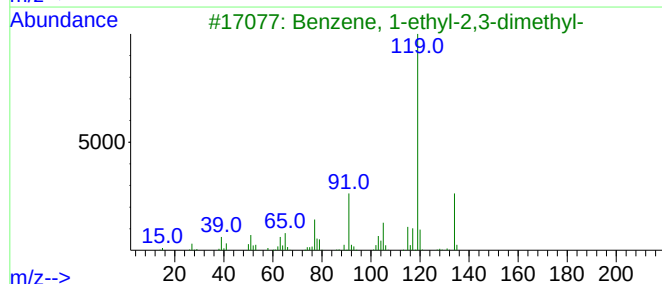
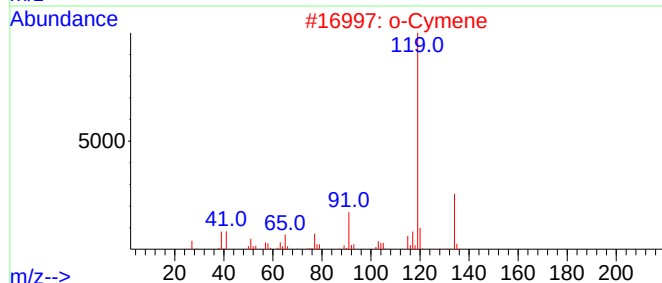
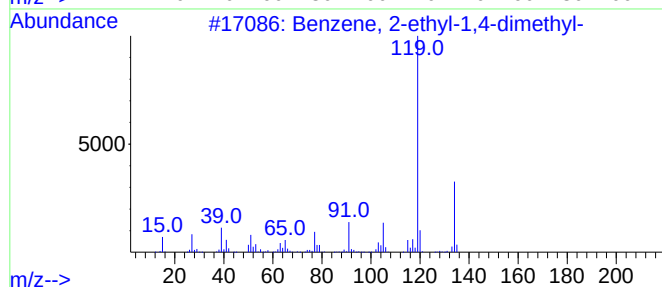
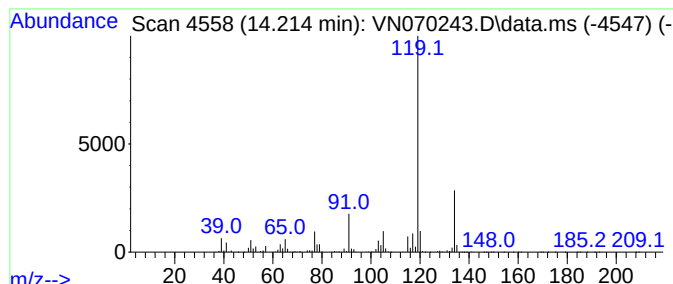
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Quant Title : SW846 8260

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

Peak Number 12 Benzene, 2-ethyl-1,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.214	29.27 ug/l	5389810	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
2			o-Cymene	134	C10H14	000527-84-4	95
3			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	94
5			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

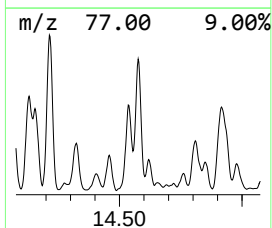
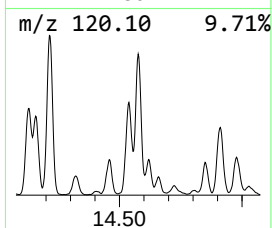
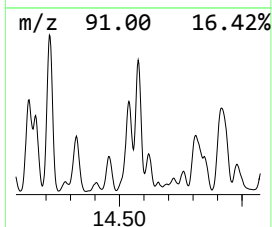
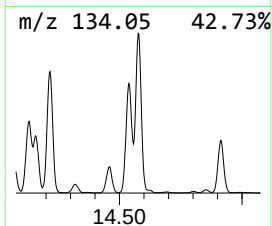
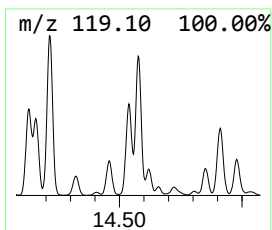
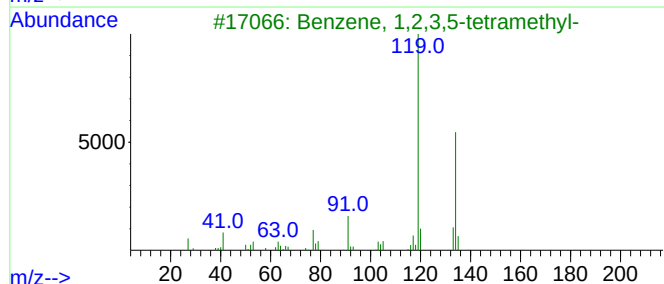
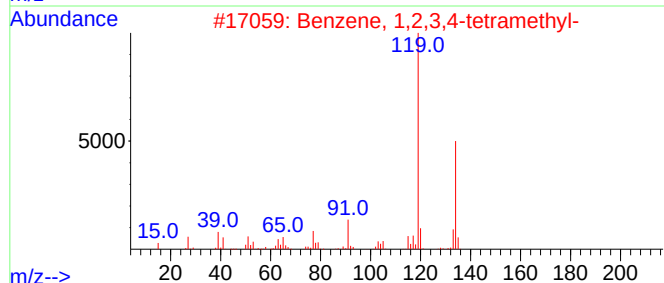
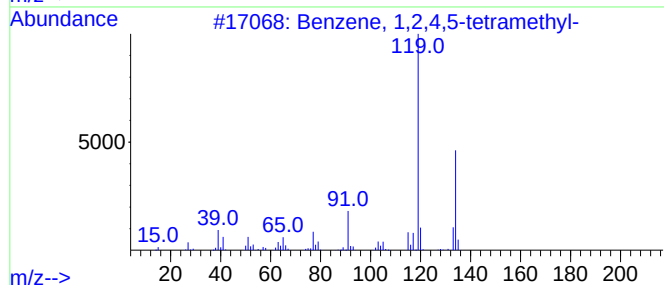
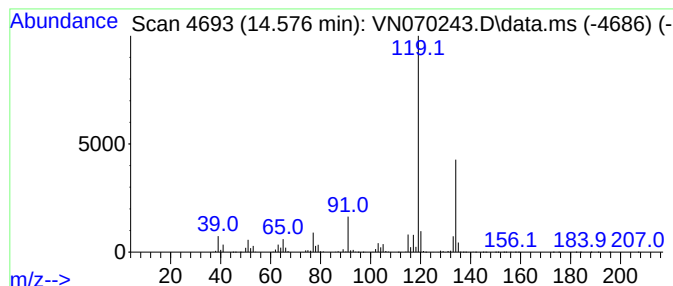
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Quant Title : SW846 8260

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

Peak Number 13 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.576	23.93 ug/l	4407200	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
4			o-Cymene	134	C10H14	000527-84-4	94
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

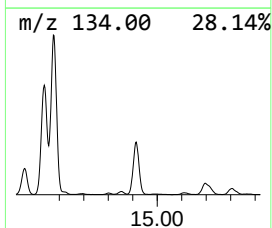
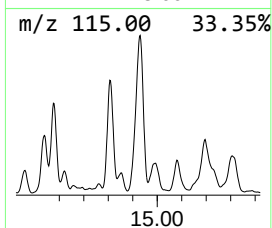
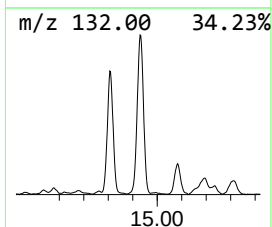
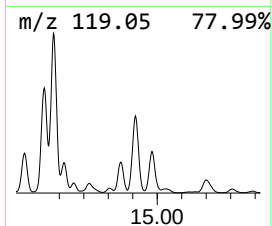
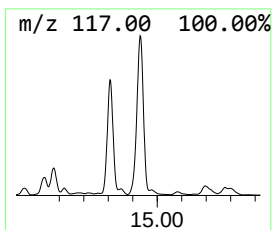
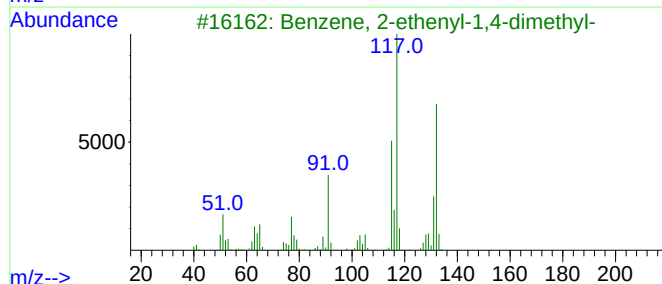
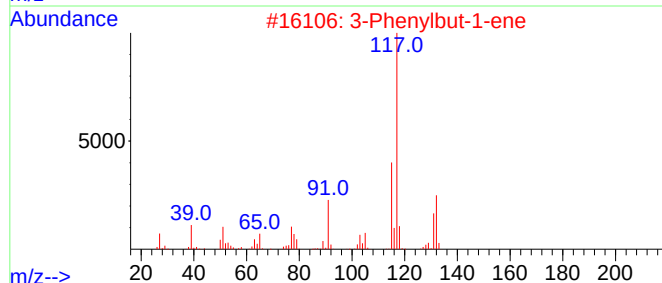
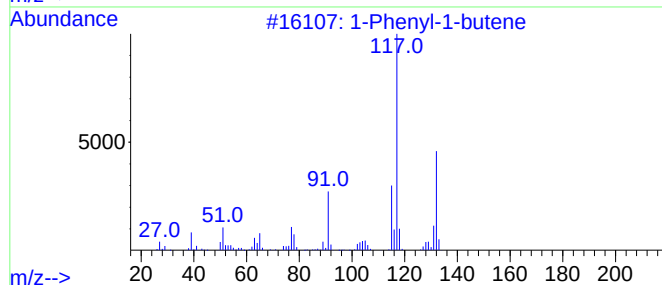
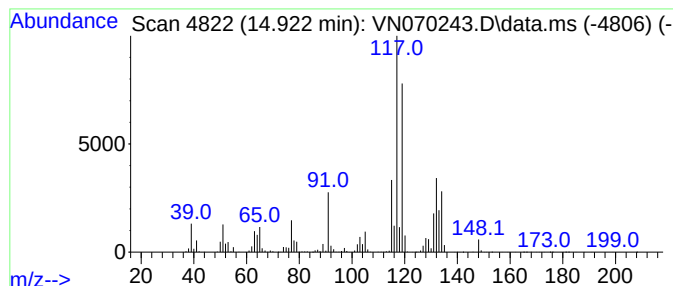
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Quant Title : SW846 8260

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

Peak Number 14 1-Phenyl-1-butene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.922	31.99 ug/l	5890970	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	87
2			3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
3			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	80
4			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	80
5			Benzene, 2-butenyl-	132	C10H12	001560-06-1	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
Data File : VN070243.D
Acq On : 20 Dec 2021 16:19
Operator : JC/MD
Sample : M5044-13
Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
DA-13-4.5

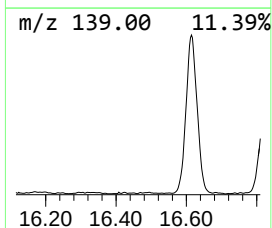
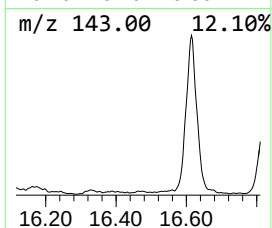
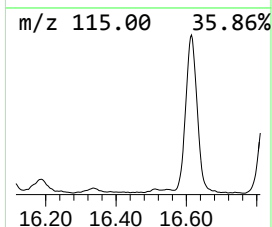
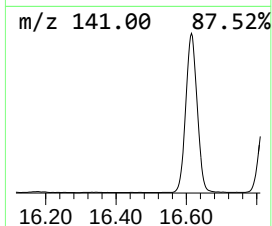
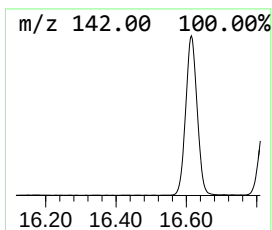
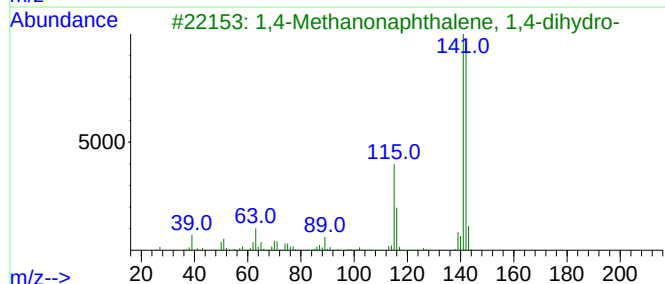
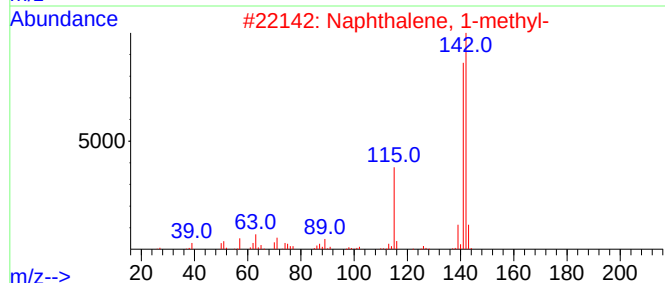
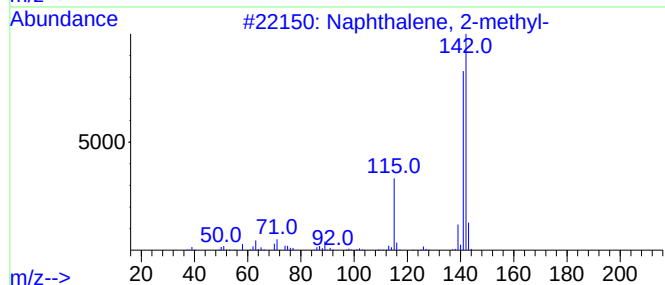
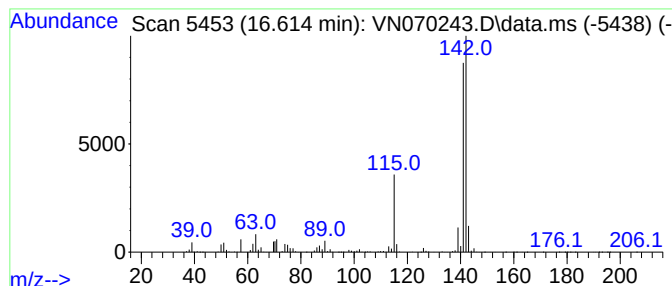
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Quant Title : SW846 8260

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

Peak Number 15 1,4-Methanonaphthalene, 1,4... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.614	20.73 ug/l	3816650	1,4-Dichlorobenzene-d4	13.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4			Benzocycloheptatriene	142	C11H10	000264-09-5	90
5			3,4-Difluorobenzaldehyde	142	C7H4F2O	034036-07-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122021\
 Data File : VN070243.D
 Acq On : 20 Dec 2021 16:19
 Operator : JC/MD
 Sample : M5044-13
 Misc : 5.89g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 DA-13-4.5

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, 3-methyl-	5.581	30.9	ug/l	1262090	1	8.080	2040860	50.0
n-Hexane	6.087	24.3	ug/l	990874	1	8.080	2040860	50.0
Pentane, 2,4-di...	7.026	43.5	ug/l	1775820	1	8.080	2040860	50.0
Pentane, 2,3-di...	8.163	74.0	ug/l	3019790	1	8.080	2040860	50.0
Hexane, 3-methyl-	8.284	64.1	ug/l	2615750	1	8.080	2040860	50.0
Pentane, 2,2,4-...	8.606	98.3	ug/l	13718500	2	8.965	6981430	50.0
Pentane, 2,3,4-...	9.877	52.5	ug/l	7327810	2	8.965	6981430	50.0
Pentane, 2,3,3-...	10.011	74.6	ug/l	10411100	2	8.965	6981430	50.0
Heptane, 3-methyl-	10.212	22.7	ug/l	3171650	2	8.965	6981430	50.0
Hexane, 2,2,4-t...	10.365	23.2	ug/l	4780410	3	11.744	10292700	50.0
Benzene, 1-ethy...	13.219	20.7	ug/l	3814110	4	13.672	9206780	50.0
Benzene, 2-ethy...	14.214	29.3	ug/l	5389810	4	13.672	9206780	50.0
Benzene, 1,2,4,...	14.576	23.9	ug/l	4407200	4	13.672	9206780	50.0
1-Phenyl-1-butene	14.922	32.0	ug/l	5890970	4	13.672	9206780	50.0
1,4-Methanonaph...	16.614	20.7	ug/l	3816650	4	13.672	9206780	50.0