

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013025\
 Data File : VN085587.D
 Acq On : 30 Jan 2025 18:18
 Operator : JC\MD
 Sample : Q1218-01 20X
 Misc : 1.05g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 BELL-25-002

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\82N011425W.M
 Title : SW846 8260

Signal : TIC: VN085587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.818	139	147	148	rBV3	10627	16614	1.61%	0.205%
2	8.165	1046	1056	1060	rBV	159763	369333	35.74%	4.564%
3	8.224	1060	1066	1077	rVB	247081	554335	53.64%	6.850%
4	8.577	1117	1126	1135	rBV	176140	396375	38.35%	4.898%
5	9.100	1205	1215	1225	rBV	381830	776331	75.12%	9.594%
6	10.565	1455	1464	1470	rBV	581262	1033489	100.00%	12.771%
7	10.624	1470	1474	1484	rVB	122597	227075	21.97%	2.806%
8	11.865	1677	1685	1698	rBV	518126	902372	87.31%	11.151%
9	12.071	1710	1720	1725	rBV3	16249	28989	2.80%	0.358%
10	12.476	1785	1789	1796	rVB3	6791	10915	1.06%	0.135%
11	12.765	1835	1838	1840	rVV2	9130	12748	1.23%	0.158%
12	12.788	1840	1842	1845	rVV3	9415	13300	1.29%	0.164%
13	12.847	1845	1852	1861	rVB	405944	701661	67.89%	8.671%
14	13.023	1877	1882	1888	rVB3	7313	13647	1.32%	0.169%
15	13.094	1888	1894	1898	rBV	17892	30822	2.98%	0.381%
16	13.159	1898	1905	1913	rVV2	87894	159625	15.45%	1.973%
17	13.218	1913	1915	1920	rVB4	9688	14507	1.40%	0.179%
18	13.312	1924	1931	1932	rBV5	7234	10537	1.02%	0.130%
19	13.394	1940	1945	1951	rVB5	20057	31057	3.01%	0.384%
20	13.482	1954	1960	1964	rBV	31084	46712	4.52%	0.577%
21	13.570	1971	1975	1979	rBV6	8820	13992	1.35%	0.173%
22	13.676	1987	1993	1996	rBV7	22033	41960	4.06%	0.519%
23	13.718	1996	2000	2003	rVV2	16447	23902	2.31%	0.295%
24	13.788	2006	2012	2020	rVV	525972	882508	85.39%	10.906%
25	13.853	2020	2023	2029	rVB3	23259	35283	3.41%	0.436%
26	13.941	2031	2038	2040	rBV6	7637	17932	1.74%	0.222%
27	13.982	2040	2045	2049	rBV3	16300	30915	2.99%	0.382%
28	14.100	2060	2065	2072	rBV	160354	264028	25.55%	3.263%
29	14.270	2087	2094	2097	rBV5	15722	34183	3.31%	0.422%
30	14.323	2099	2103	2107	rVB4	18558	25784	2.49%	0.319%
31	14.365	2108	2110	2116	rVB6	15898	22313	2.16%	0.276%
32	14.435	2117	2122	2128	rVB6	24755	41062	3.97%	0.507%
33	14.500	2128	2133	2137	rBV7	7574	16883	1.63%	0.209%
34	14.582	2140	2147	2150	rBV5	24871	52864	5.12%	0.653%
35	14.623	2150	2154	2157	rVV3	47360	65358	6.32%	0.808%
36	14.659	2157	2160	2164	rVB2	17813	21973	2.13%	0.272%

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37	14.729	2169	2172	2176	rVB3	29826	37959	3.67%	0.469%
38	14.788	2176	2182	2188	rVB8	16008	34804	3.37%	0.430%
39	14.847	2188	2192	2195	rBV6	13096	24971	2.42%	0.309%
40	14.959	2201	2211	2217	rBV3	143622	267067	25.84%	3.300%
41	15.053	2218	2227	2229	rBV6	48511	126858	12.27%	1.568%
42	15.217	2250	2255	2260	rVB4	27420	54822	5.30%	0.677%
43	15.317	2267	2272	2277	rVV6	20066	35235	3.41%	0.435%
44	15.500	2299	2303	2312	rVB8	25947	60409	5.85%	0.747%
45	15.588	2313	2318	2323	rBV4	25950	50295	4.87%	0.622%
46	15.688	2332	2335	2340	rVB5	9543	17262	1.67%	0.213%
47	15.741	2340	2344	2348	rBV7	10101	14507	1.40%	0.179%
48	15.829	2354	2359	2370	rVB2	89537	180502	17.47%	2.231%
49	15.941	2370	2378	2385	rBV10	22011	60679	5.87%	0.750%
50	16.023	2387	2392	2397	rVB8	7523	12086	1.17%	0.149%
51	16.117	2403	2408	2410	rBV6	8505	13544	1.31%	0.167%
52	16.164	2411	2416	2422	rVB6	30628	65191	6.31%	0.806%
53	16.323	2437	2443	2444	rBV6	6490	11513	1.11%	0.142%
54	16.494	2468	2472	2477	rVV7	11167	23261	2.25%	0.287%
55	16.535	2477	2479	2486	rVB8	14122	20742	2.01%	0.256%
56	16.706	2503	2508	2515	rVB7	18288	39071	3.78%	0.483%

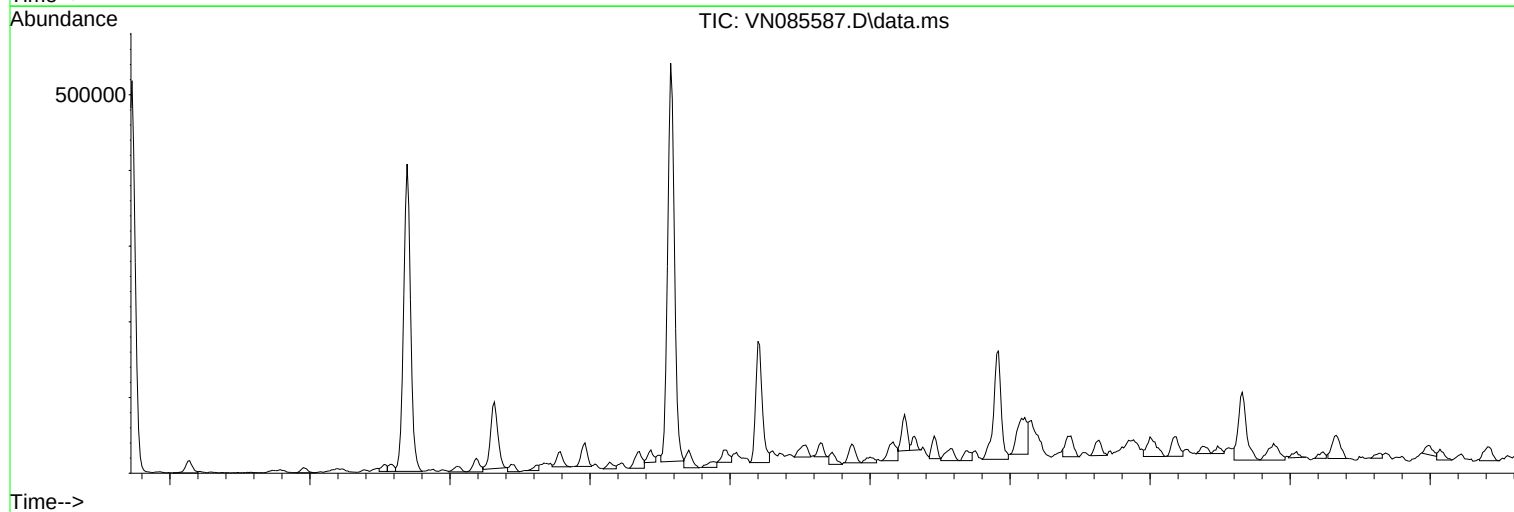
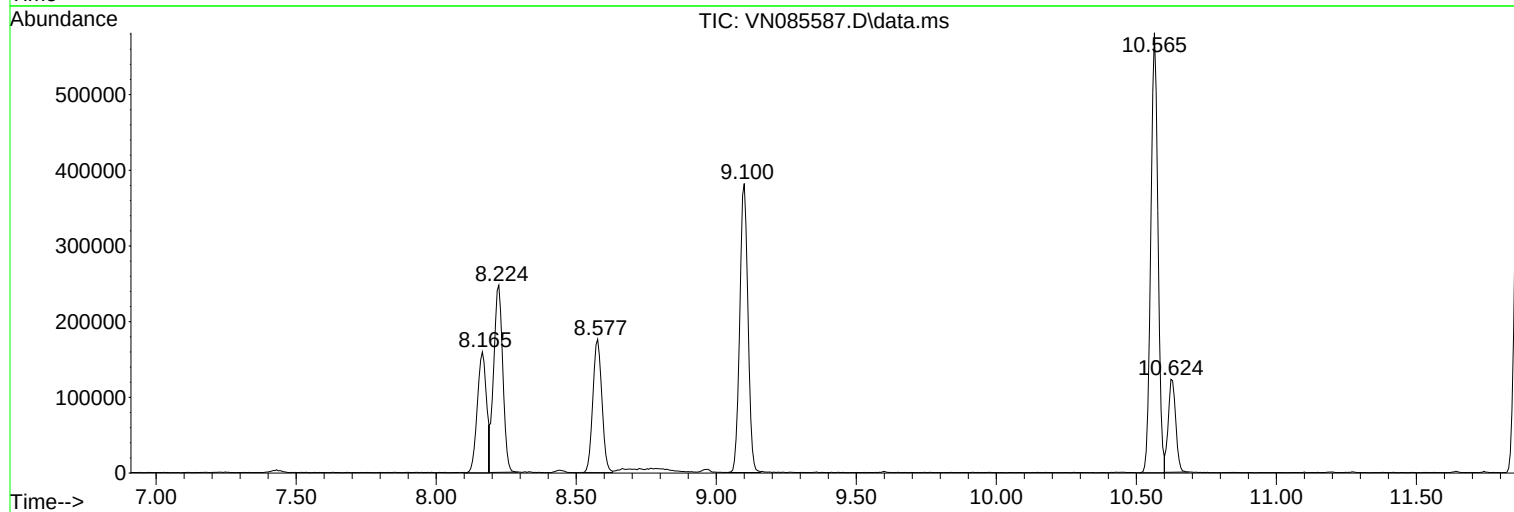
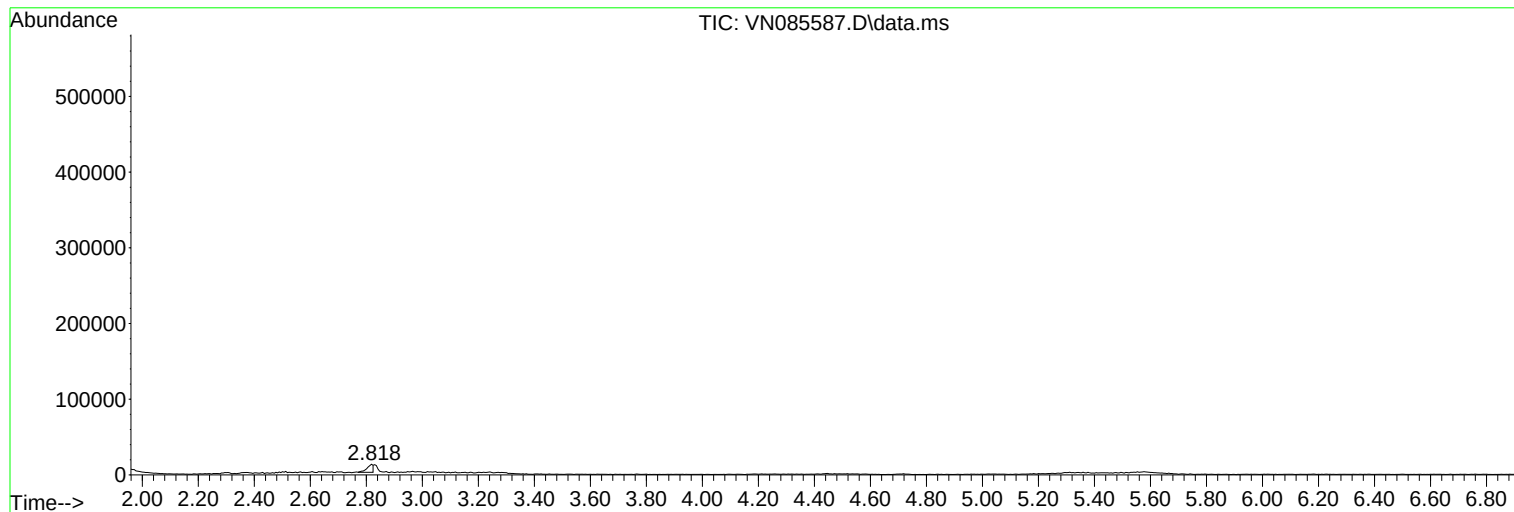
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_N
ClientSampleId :
BELL-25-002

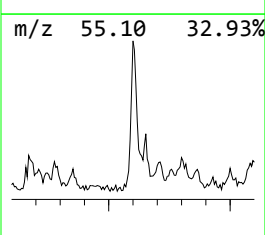
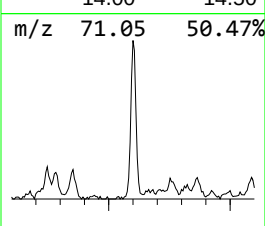
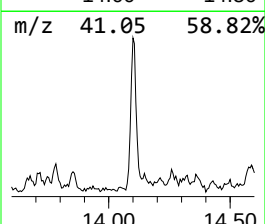
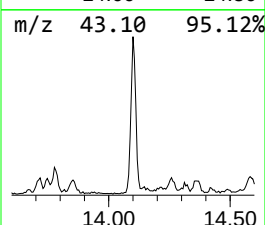
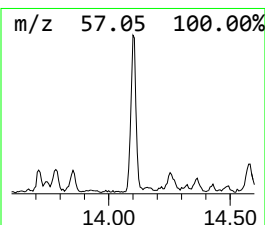
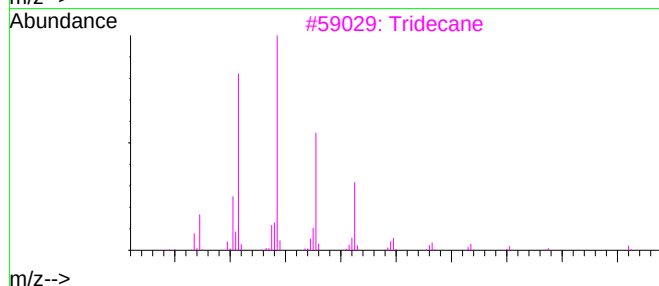
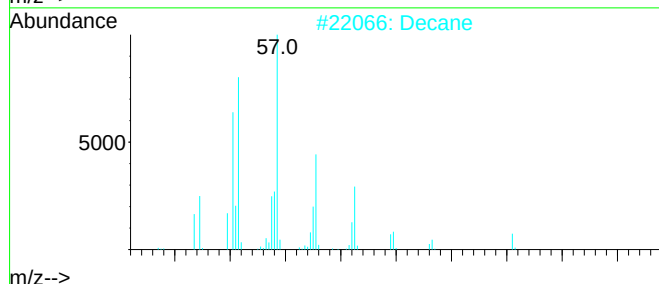
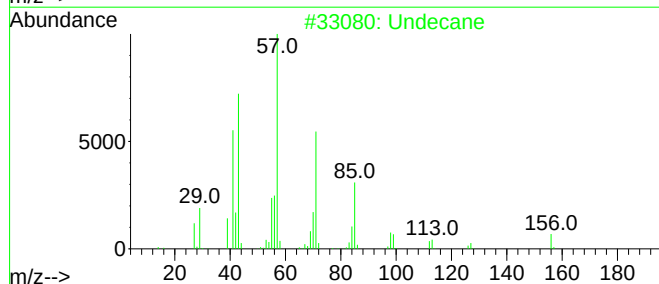
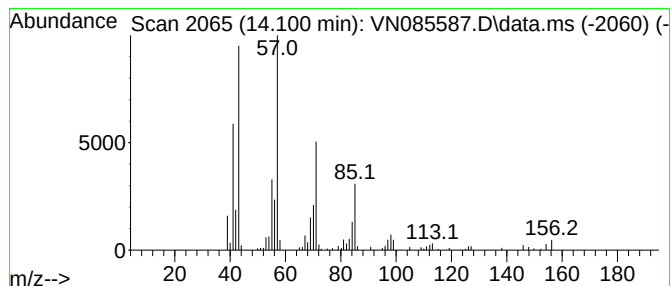
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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

Peak Number 1 Undecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.100	14.96 ug/l	264028	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane	156	C11H24	001120-21-4	93
2	Decane	142	C10H22	000124-18-5	78
3	Tridecane	184	C13H28	000629-50-5	59
4	Hexadecane	226	C16H34	000544-76-3	53
5	Heptacosyl acetate	438	C29H58O2	1000351-78-2	53



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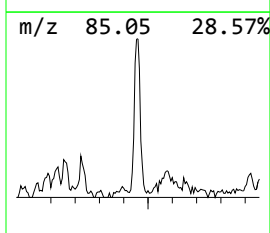
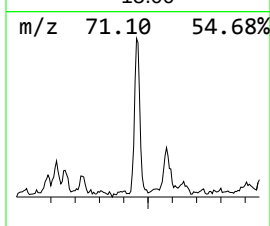
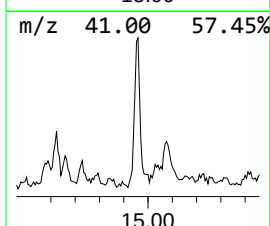
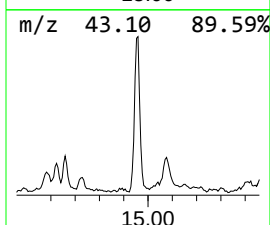
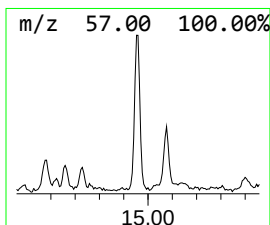
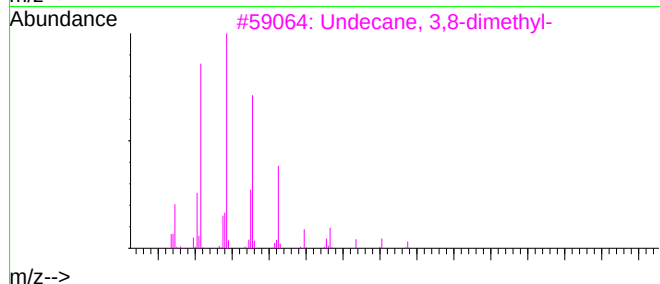
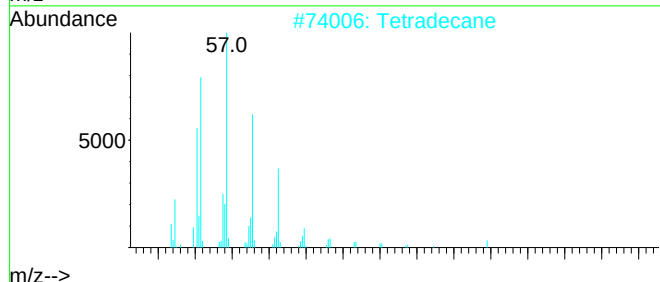
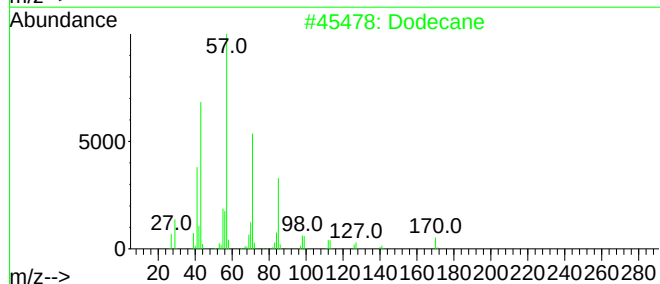
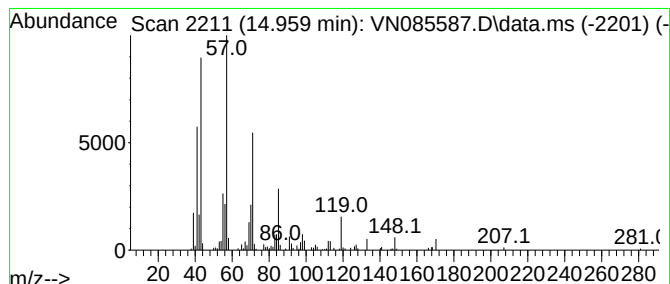
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Quant Title : SW846 8260

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

Peak Number 2 Dodecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.959	15.13 ug/l	267067	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	92
2	Tetradecane	198	C14H30	000629-59-4	64
3	Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	59
4	Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	58
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

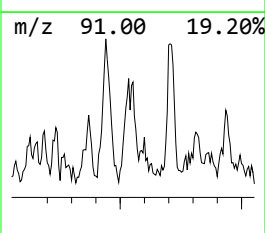
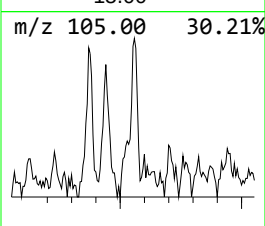
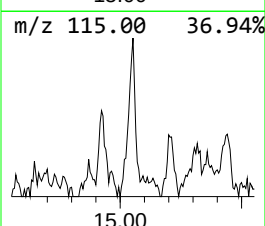
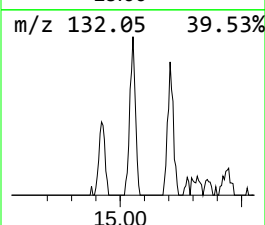
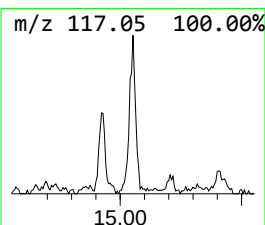
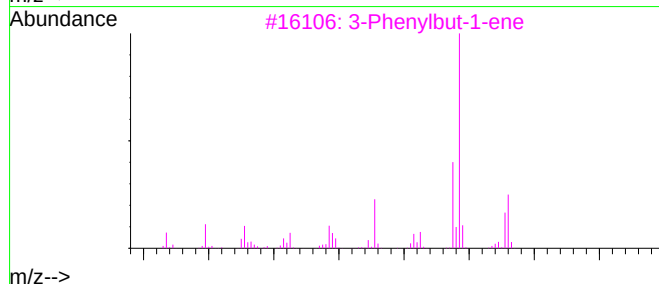
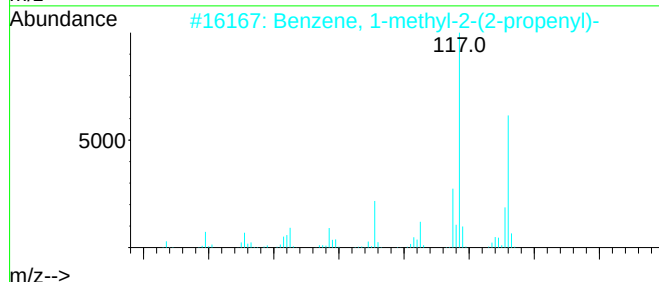
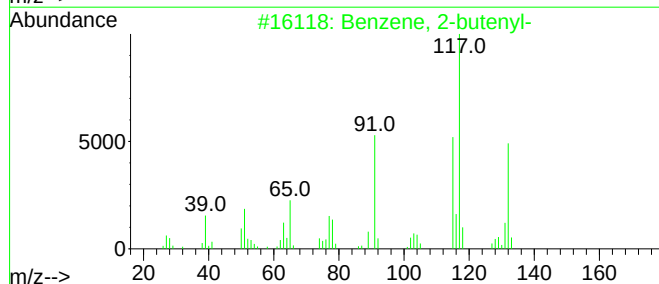
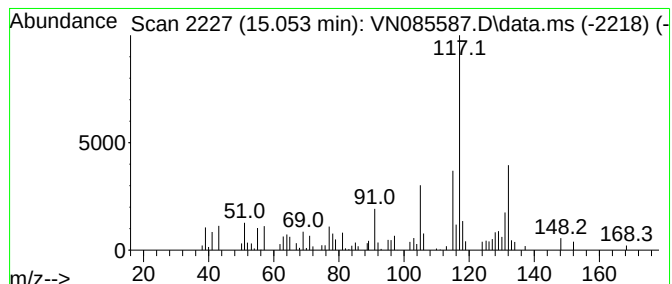
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 2-butenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	7.19 ug/l	126858	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-butenyl-	132	C10H12	001560-06-1	90
2	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	87
4	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	81
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	81



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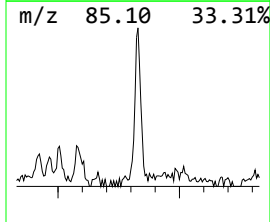
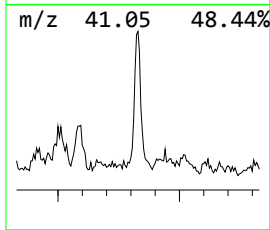
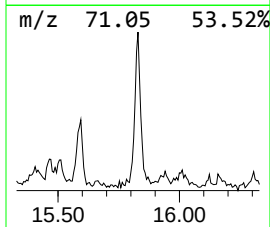
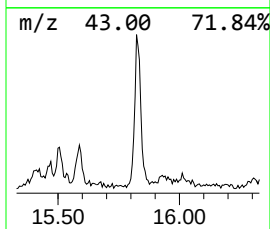
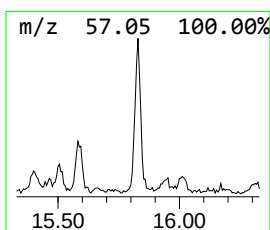
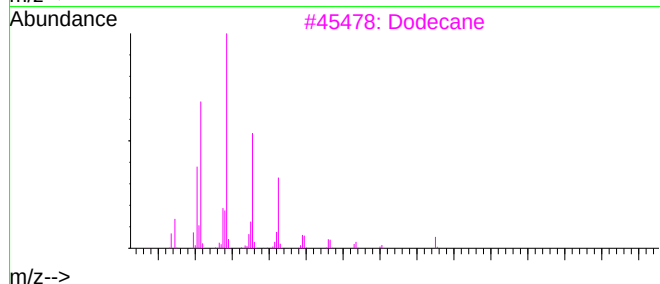
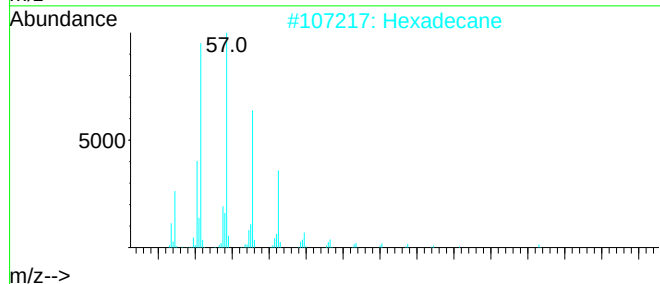
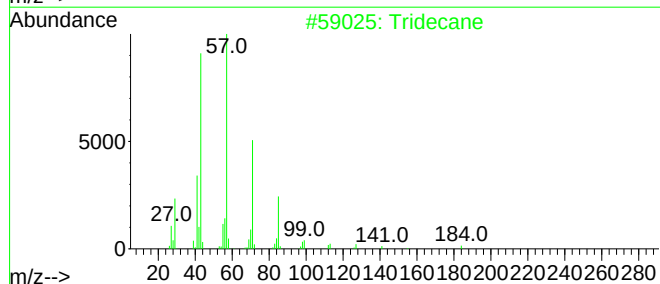
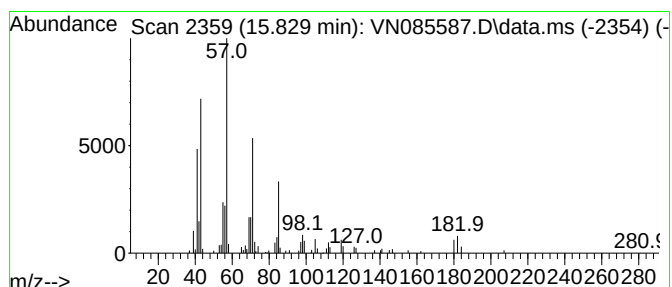
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N011425W.M
Quant Title : SW846 8260

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

Peak Number 4 Tridecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.829	10.23 ug/l	180502	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	76
2	Hexadecane	226	C16H34	000544-76-3	64
3	Dodecane	170	C12H26	000112-40-3	64
4	Tetradecane	198	C14H30	000629-59-4	59
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Undecane	14.100	15.0	ug/l	264028	4	13.788	882508	50.0
Dodecane	14.959	15.1	ug/l	267067	4	13.788	882508	50.0
Benzene, 2-bute...	15.053	7.2	ug/l	126858	4	13.788	882508	50.0
Tridecane	15.829	10.2	ug/l	180502	4	13.788	882508	50.0