

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091919\
 Data File : VX012524.D
 Acq On : 19 Sep 2019 13:37
 Operator : JC/SP
 Sample : K4888-02
 Misc : 6.11g/10mL/100uL/10mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 980-B-1-(24)

Integration Parameters: RTEINT.P

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

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

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

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.064	25	29	42	rBV	343546	405840	44.89%	6.450%
2	1.259	58	61	69	rBV2	16393	21920	2.42%	0.348%
3	1.667	104	128	129	rBV5	33128	140455	15.54%	2.232%
4	3.009	339	348	357	rBV	11761	29469	3.26%	0.468%
5	5.490	742	755	769	rBV	95844	274844	30.40%	4.368%
6	5.642	769	780	794	rVV	198381	559733	61.92%	8.896%
7	6.051	837	847	858	rBV	120915	315444	34.89%	5.013%
8	6.849	968	978	989	rBV	284631	678057	75.01%	10.776%
9	8.709	1275	1283	1293	rBV	578518	903996	100.00%	14.367%
10	9.331	1379	1385	1390	rBV	29184	43611	4.82%	0.693%
11	10.111	1507	1513	1523	rBV	551991	760308	84.11%	12.083%
12	11.135	1675	1681	1689	rBV	450380	579883	64.15%	9.216%
13	12.074	1830	1835	1842	rVB	566052	703403	77.81%	11.179%
14	12.476	1897	1901	1905	rVB5	8186	10851	1.20%	0.172%
15	13.318	2036	2039	2041	rBV2	19123	21472	2.38%	0.341%
16	13.440	2056	2059	2060	rBV3	8043	10073	1.11%	0.160%
17	14.086	2162	2165	2169	rBV	29049	33785	3.74%	0.537%
18	14.519	2234	2236	2239	rBV4	6721	9231	1.02%	0.147%
19	14.616	2249	2252	2256	rVB4	9333	11530	1.28%	0.183%
20	14.665	2257	2260	2266	rVB6	17422	21837	2.42%	0.347%
21	14.805	2279	2283	2287	rVB	75705	82413	9.12%	1.310%
22	14.897	2293	2298	2301	rBV7	10200	17820	1.97%	0.283%
23	15.238	2351	2354	2356	rBV4	9838	11843	1.31%	0.188%
24	15.269	2356	2359	2363	rVV2	39195	52334	5.79%	0.832%
25	15.336	2367	2370	2374	rVB3	20060	25255	2.79%	0.401%
26	15.433	2384	2386	2391	rBV6	6638	11545	1.28%	0.183%
27	15.555	2401	2406	2412	rVB	148177	210043	23.23%	3.338%
28	15.964	2468	2473	2478	rBV6	12456	27937	3.09%	0.444%
29	16.104	2493	2496	2500	rVB3	20404	31035	3.43%	0.493%
30	16.189	2501	2510	2514	rBV8	18586	53885	5.96%	0.856%
31	16.372	2537	2540	2546	rBV8	6405	13689	1.51%	0.218%
32	16.457	2548	2554	2562	rVB	127152	218626	24.18%	3.475%

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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

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Title : SW846 8260

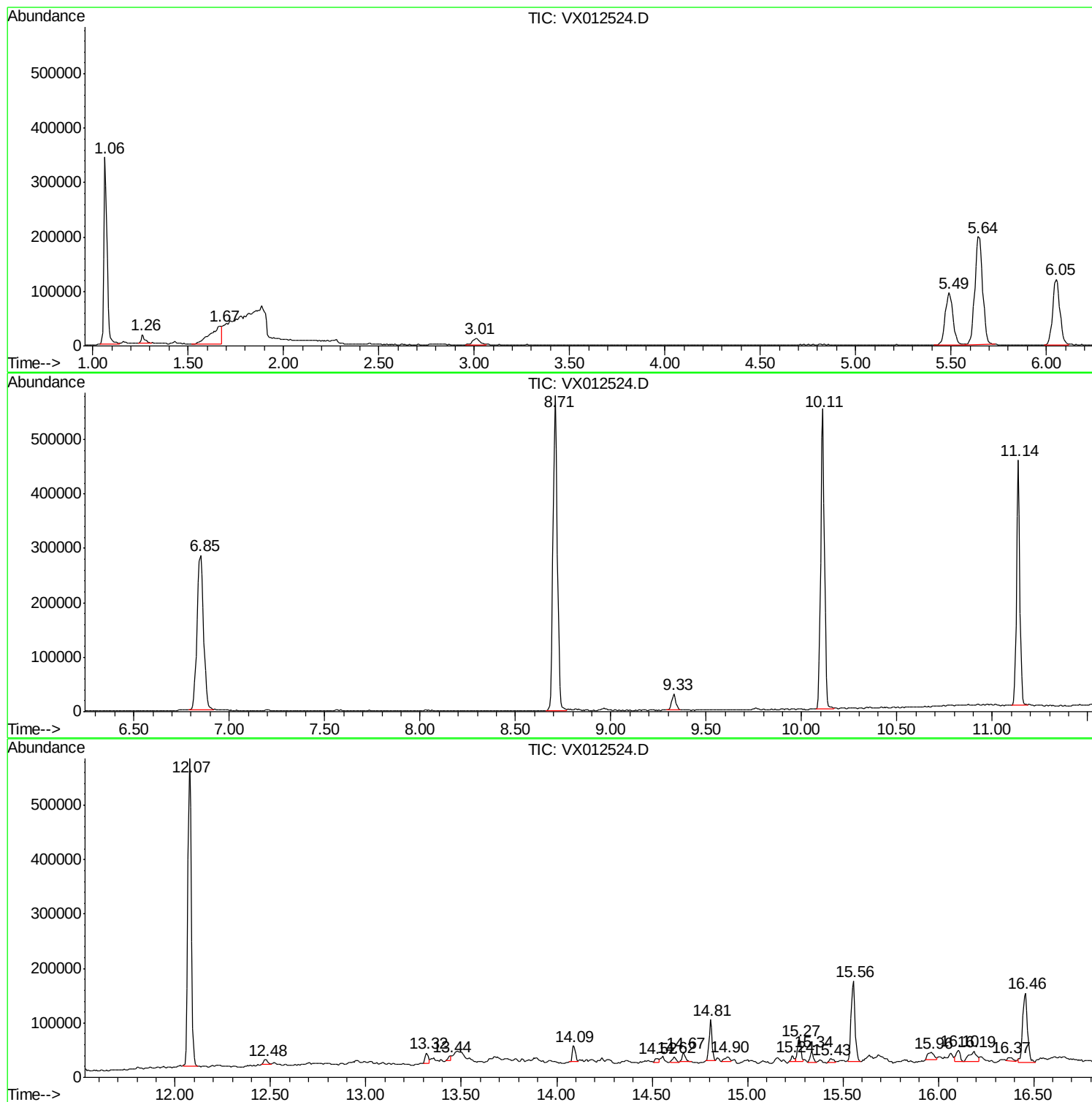
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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MSVOA_X
ClientSampled :
980-B-1-(24)

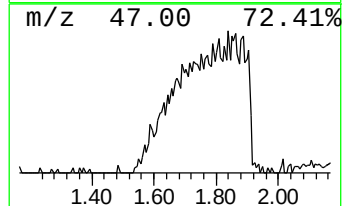
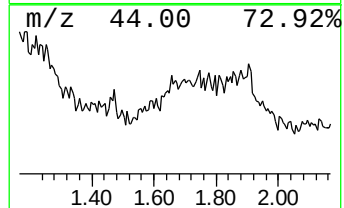
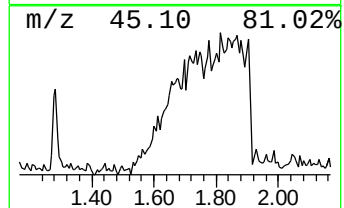
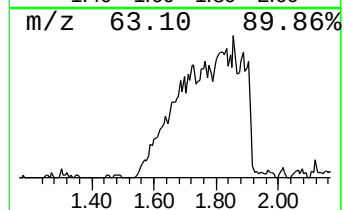
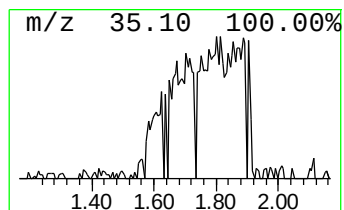
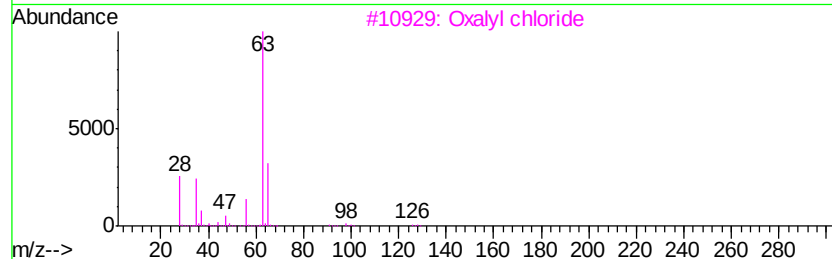
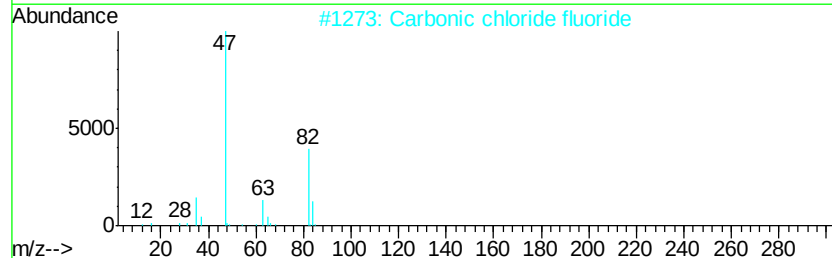
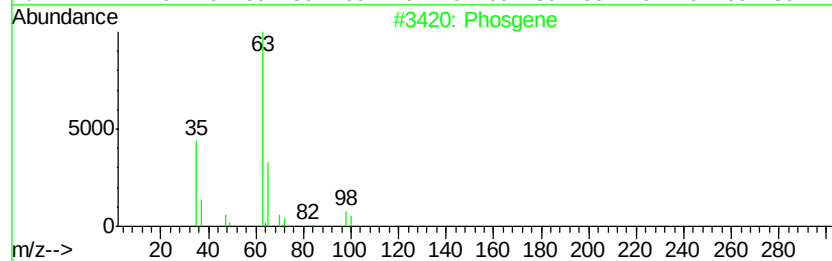
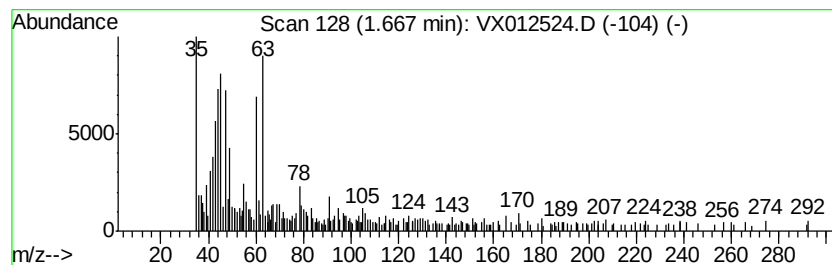
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 2 Phosgene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	12.55 ug/l	140455	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosgene		98	CCl ₂ O	000075-44-5	50
2	Carbonic chloride fluoride		82	CClFO	000353-49-1	33
3	Oxalyl chloride		126	C ₂ Cl ₂ O ₂	000079-37-8	27
4	Trivinylphosphine oxide		128	C ₆ H ₉ OP	013699-67-7	25
5	Divinyldithiophosphinic acid		150	C ₄ H ₇ PS ₂	085417-00-1	25



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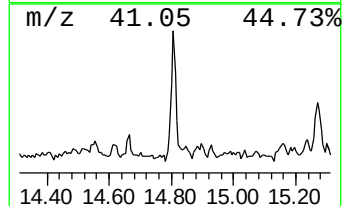
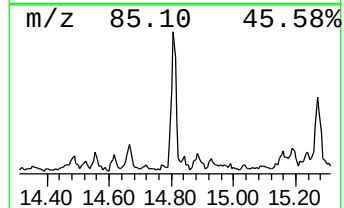
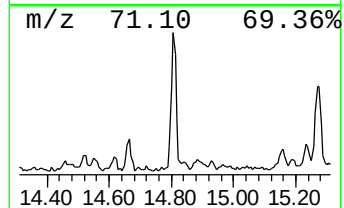
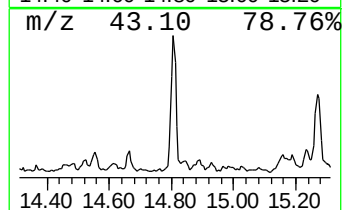
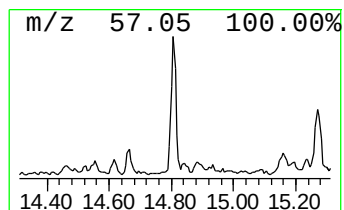
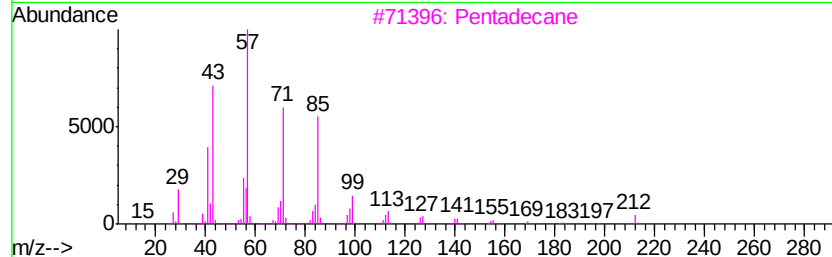
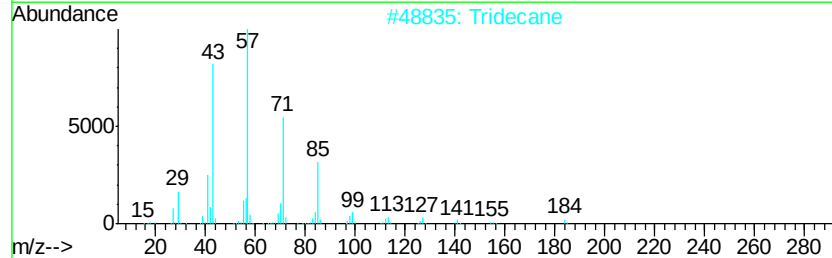
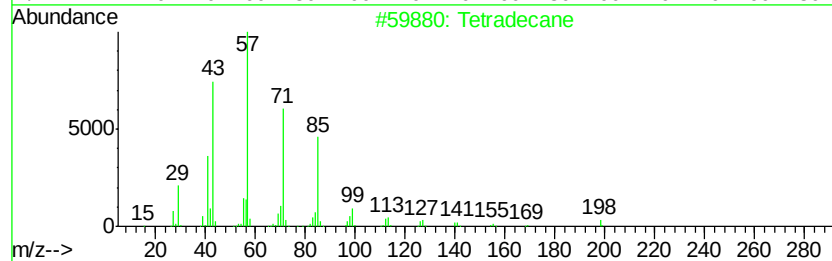
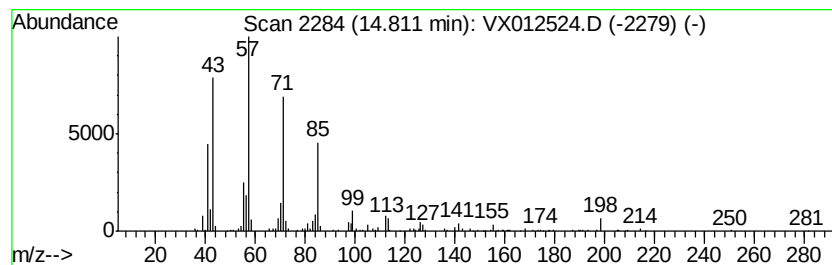
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	5.86 ug/l	82413	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	96
2		Tridecane	184	C13H28	000629-50-5	90
3		Pentadecane	212	C15H32	000629-62-9	90
4		Nonadecane	268	C19H40	000629-92-5	90
5		Hexadecane	226	C16H34	000544-76-3	86



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ClientSampleId :
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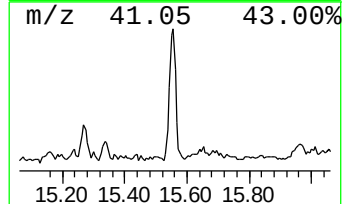
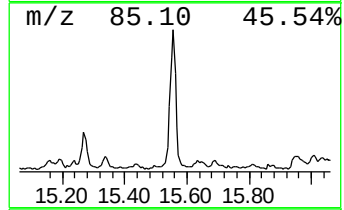
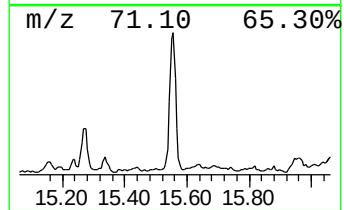
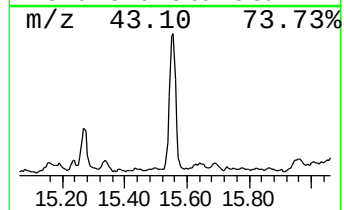
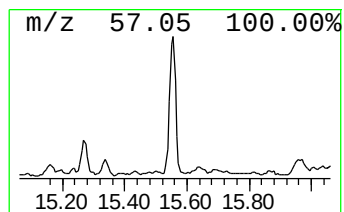
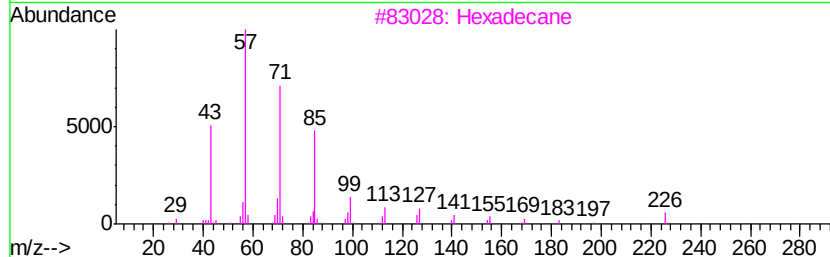
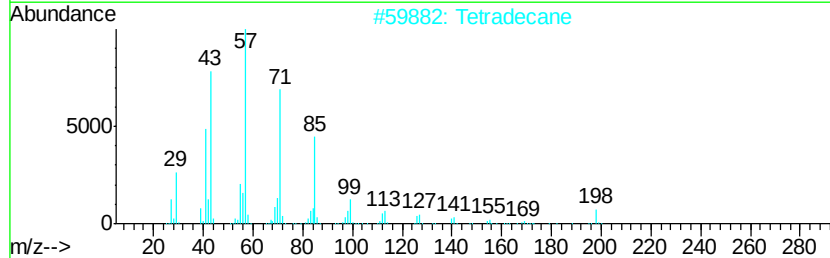
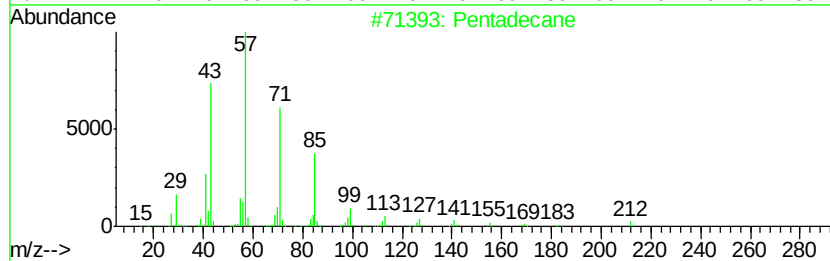
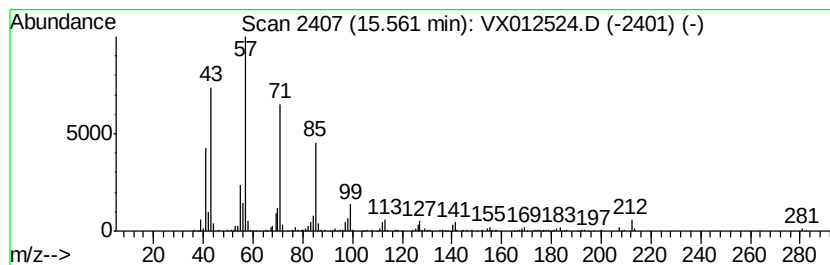
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Quant Title : SW846 8260

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

Peak Number 4 Pentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	14.93 ug/l	210043	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	97
2	Tetradecane		198	C14H30	000629-59-4	91
3	Hexadecane		226	C16H34	000544-76-3	91
4	Heptadecane, 2,6,10,15-tetramethyl-		296	C21H44	054833-48-6	91
5	Tetracosane		338	C24H50	000646-31-1	87



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 ALS Vial : 9 Sample Multiplier: 1

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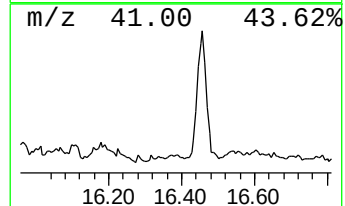
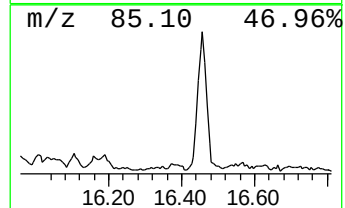
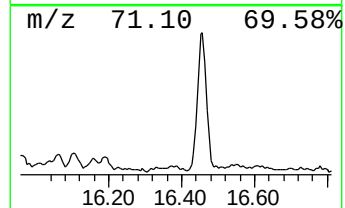
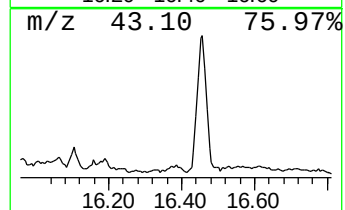
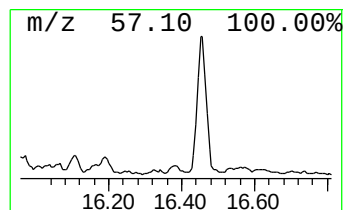
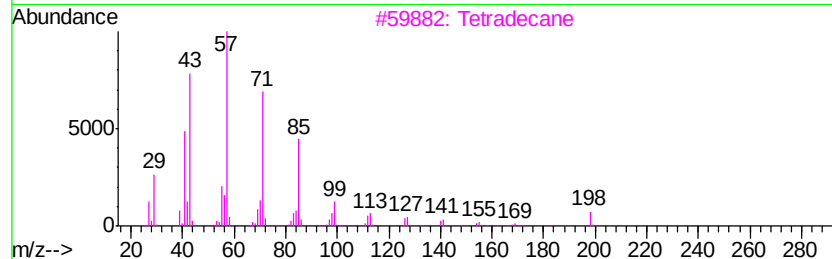
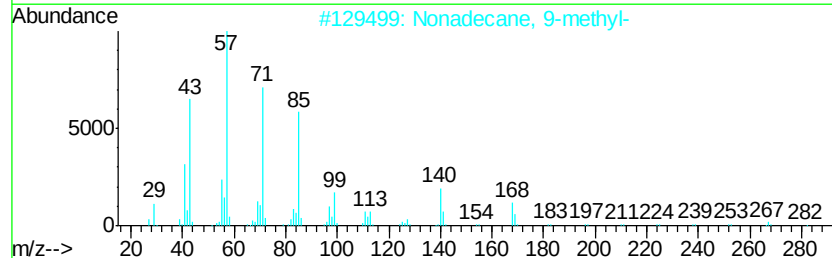
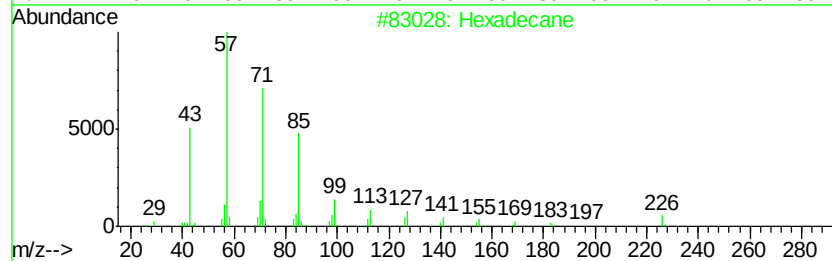
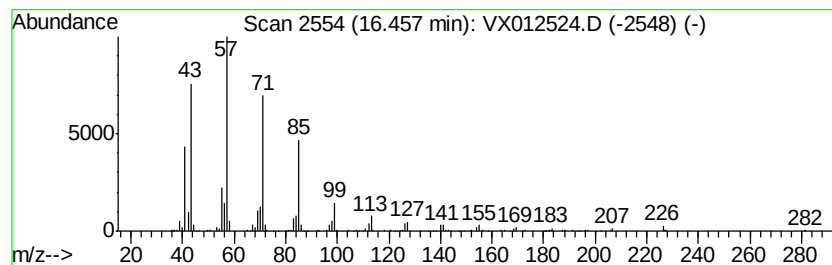
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	15.54 ug/l	218626	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	97
2	Nonadecane, 9-methyl-		282	C20H42	013287-24-6	93
3	Tetradecane		198	C14H30	000629-59-4	91
4	Heptadecane		240	C17H36	000629-78-7	91
5	Pentadecane		212	C15H32	000629-62-9	91



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phosgene	1.67	12.6	ug/l	140455	1	5.65	559733	50.0
Tetradecane	14.81	5.9	ug/l	82413	4	12.07	703403	50.0
Pentadecane	15.56	14.9	ug/l	210043	4	12.07	703403	50.0
Hexadecane	16.46	15.5	ug/l	218626	4	12.07	703403	50.0