

Data Path : Z:\VOASRV\HPCHEM1\MSVOA Y\DATA\VY110819\
 Data File : VY000624.D
 Acq On : 08 Nov 2019 17:47
 Operator : SY/MD
 Sample : K5723-11
 Misc : 7.08G/5ML/MSVOA Y/SOIL
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 9-D

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_Y\METHODS\82Y103019S.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	2.212	75	78	80	rBV3	1567	2187	1.30%	0.173%
2	2.316	90	95	96	rBV2	1878	2571	1.52%	0.203%
3	2.846	176	182	187	rBV5	1152	2286	1.35%	0.181%
4	3.529	289	294	297	rBV4	1108	1853	1.10%	0.147%
5	4.724	483	490	499	rBV5	2715	7620	4.52%	0.603%
6	5.754	651	659	660	rBV4	5089	10216	6.05%	0.808%
7	6.998	856	863	867	rBV2	1088	2334	1.38%	0.185%
8	7.730	974	983	989	rBV2	23907	54520	32.31%	4.314%
9	7.803	989	995	1003	rVB2	44580	99182	58.78%	7.847%
10	8.150	1043	1052	1062	rBV2	26285	54435	32.26%	4.307%
11	8.699	1133	1142	1153	rVB2	64324	131460	77.91%	10.401%
12	10.180	1379	1385	1393	rVV	98401	168737	100.00%	13.351%
13	11.491	1593	1600	1608	rBV	86807	142260	84.31%	11.256%
14	12.479	1756	1762	1772	rVB	65545	102293	60.62%	8.094%
15	13.302	1891	1897	1901	rBV5	7497	13126	7.78%	1.039%
16	13.424	1910	1917	1926	rBV	83941	130451	77.31%	10.321%
17	13.692	1956	1961	1966	rVB3	3012	5296	3.14%	0.419%
18	13.966	2001	2006	2014	rVB8	1254	3199	1.90%	0.253%
19	14.296	2057	2060	2064	rBV4	1528	1719	1.02%	0.136%
20	14.381	2069	2074	2078	rBV3	1487	2799	1.66%	0.221%
21	14.814	2141	2145	2146	rBV3	1687	1745	1.03%	0.138%
22	14.838	2146	2149	2151	rVB4	1475	1788	1.06%	0.141%
23	14.930	2162	2164	2168	rVB4	1736	2075	1.23%	0.164%
24	15.021	2177	2179	2184	rBV4	1167	2150	1.27%	0.170%
25	15.155	2199	2201	2204	rVB3	2349	2058	1.22%	0.163%
26	15.216	2204	2211	2213	rBV6	2810	4998	2.96%	0.395%
27	15.265	2213	2219	2224	rVV2	33823	55349	32.80%	4.379%
28	15.332	2224	2230	2237	rVB2	29964	51754	30.67%	4.095%
29	15.417	2237	2244	2253	rBV5	42789	93678	55.52%	7.412%
30	15.503	2255	2258	2262	rBV7	2502	4210	2.50%	0.333%
31	15.704	2290	2291	2294	rBV3	1916	1746	1.03%	0.138%
32	15.777	2301	2303	2307	rVB5	2412	3254	1.93%	0.257%
33	15.807	2307	2308	2312	rBV3	2381	3136	1.86%	0.248%
34	15.862	2315	2317	2318	rBV	3363	2378	1.41%	0.188%

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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 >
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Title : SW846 8260

35	15.881	2318	2320	2322	rVV3	2832	2410	1.43%	0.191%
36	15.960	2331	2333	2336	rVB4	2277	2362	1.40%	0.187%
37	16.009	2338	2341	2348	rVB7	5488	10507	6.23%	0.831%
38	16.094	2353	2355	2360	rVB5	6620	8393	4.97%	0.664%
39	16.155	2360	2365	2370	rBV8	7655	14671	8.69%	1.161%
40	16.356	2393	2398	2404	rBV3	24023	43296	25.66%	3.426%
41	16.466	2411	2416	2418	rBV6	3827	6764	4.01%	0.535%
42	16.862	2478	2481	2484	rBV5	2788	4272	2.53%	0.338%
43	16.917	2488	2490	2492	rBV3	2008	2345	1.39%	0.186%

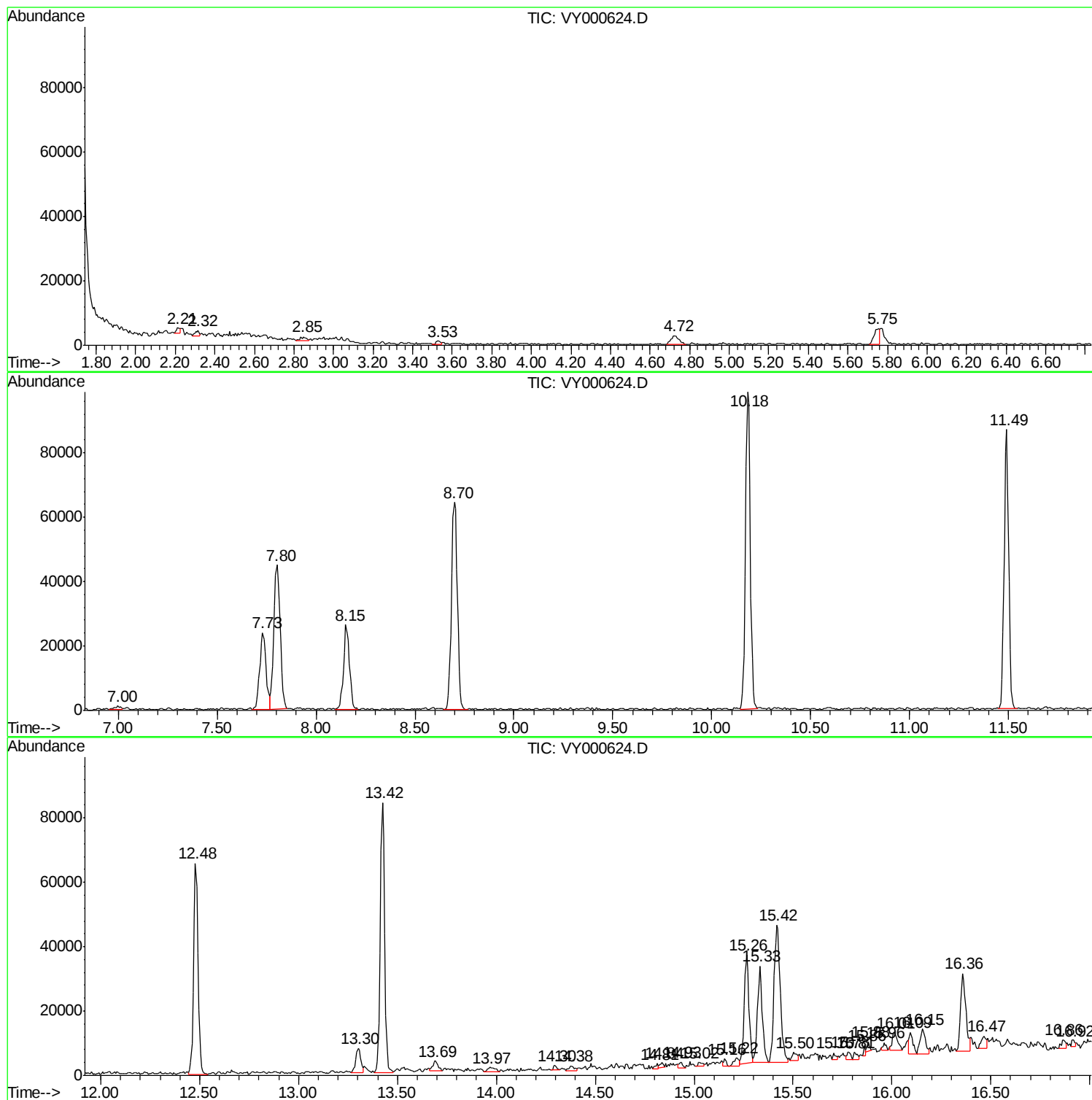
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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



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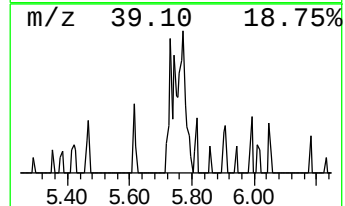
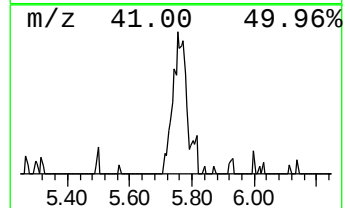
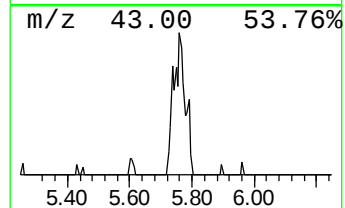
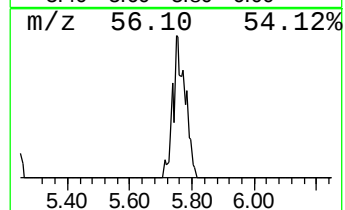
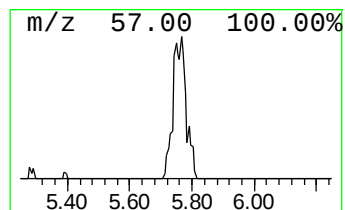
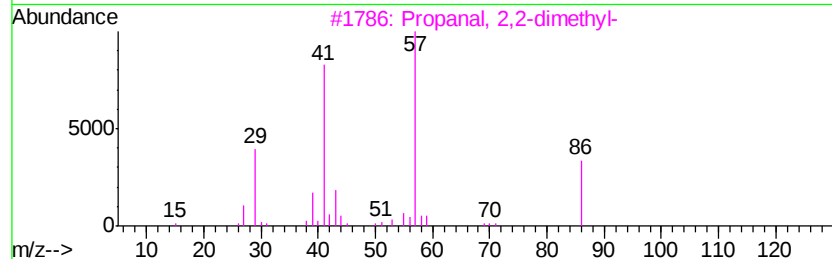
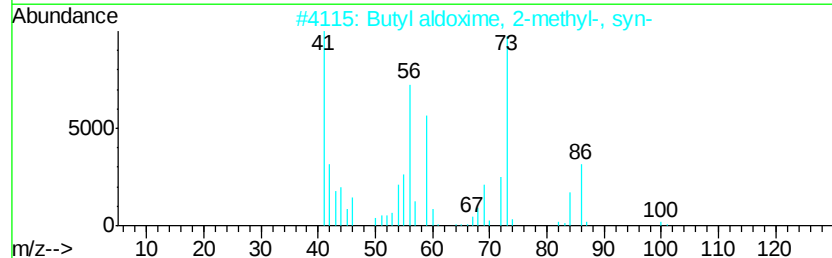
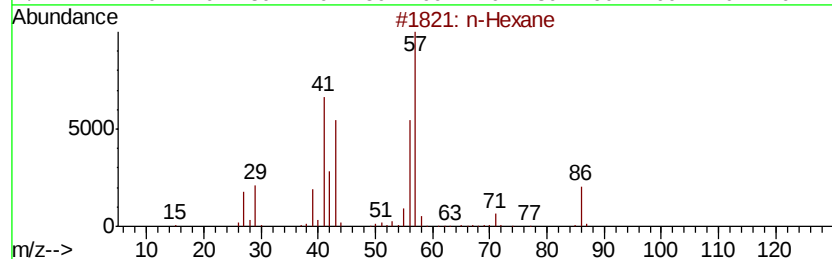
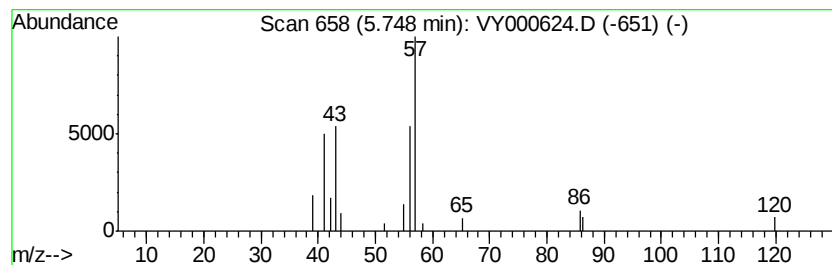
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.75	5.15 ug/l	10216	Pentafluorobenzene	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	86
2		Butyl aldoxime, 2-methyl-, syn-	101	C5H11NO	049805-56-3	56
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	37
4		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	9
5		Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9



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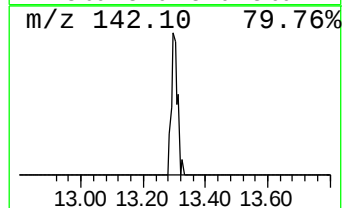
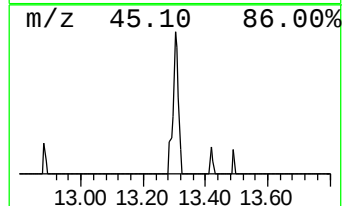
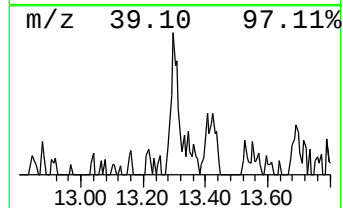
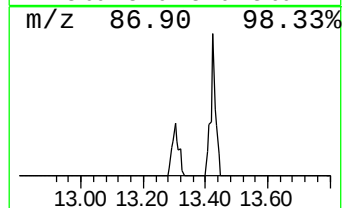
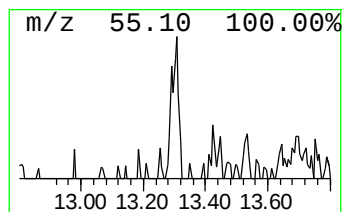
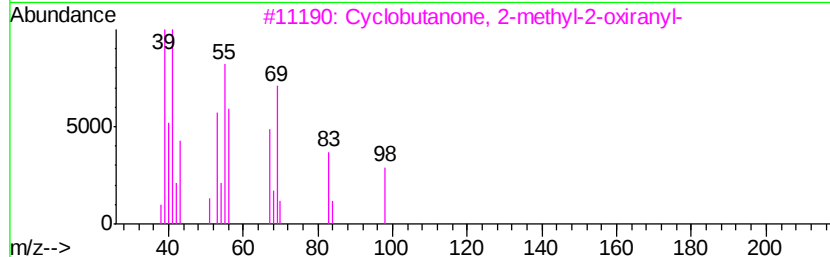
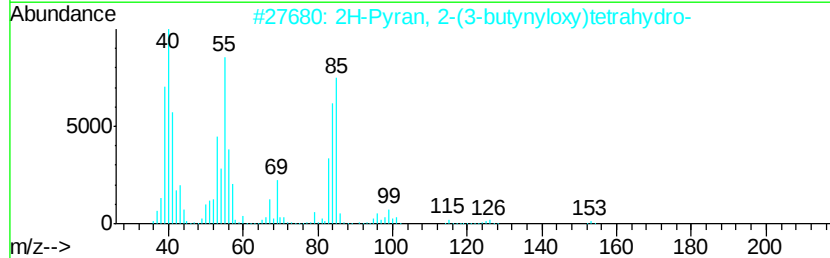
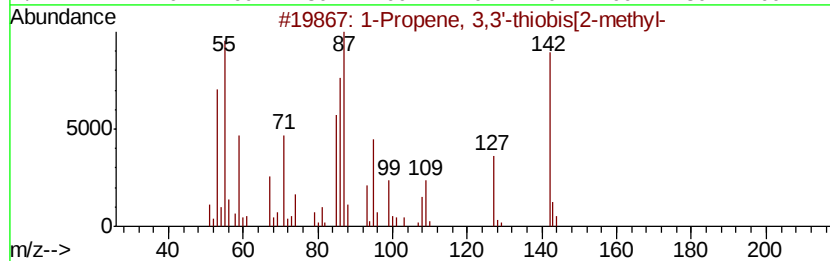
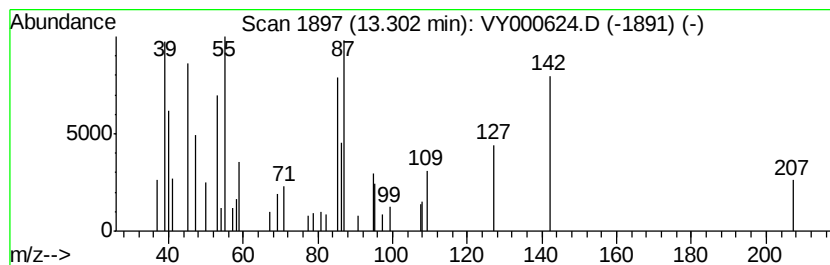
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Peak Number 2 unknown13.30 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.30	5.03 ug/l	13126	1,4-Dichlorobenzene-d4	13.42

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	38
2			2H-Pyran, 2-(3-butynloxy)tetrah...	154	C9H14O2	040365-61-5	25
3			Cyclobutanone, 2-methyl-2-oxiranyl-	126	C7H10O2	075314-19-1	25
4			Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	17
5			Cyclopropene	40	C3H4	002781-85-3	16



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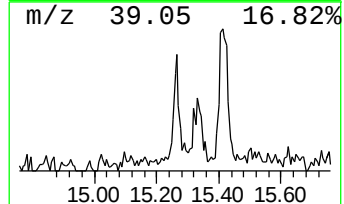
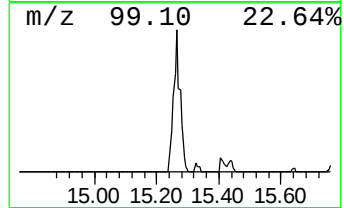
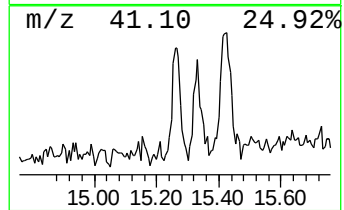
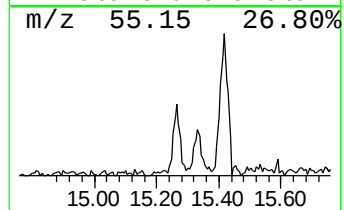
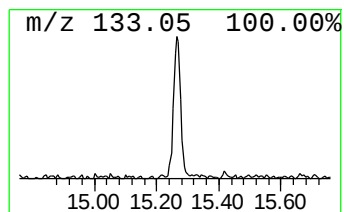
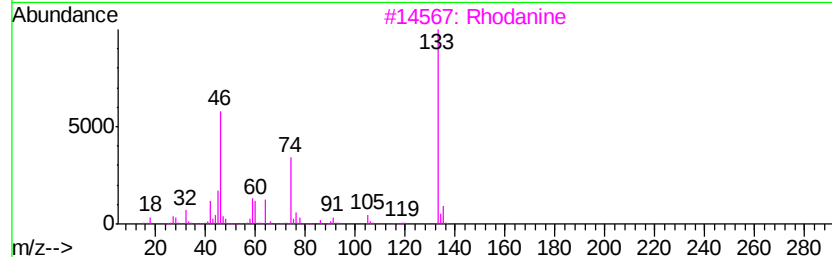
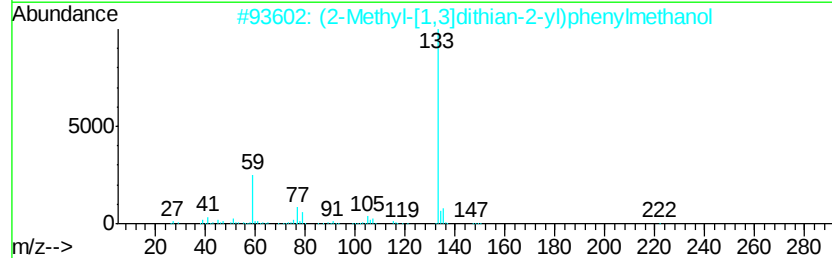
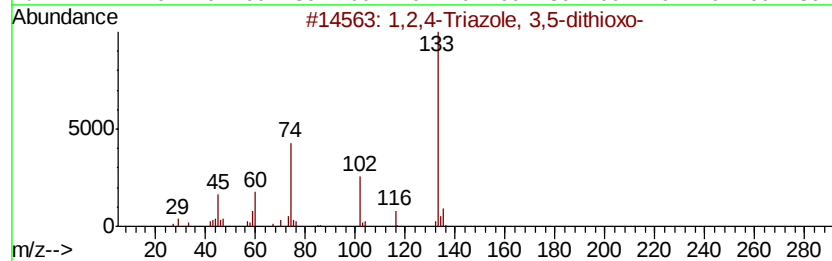
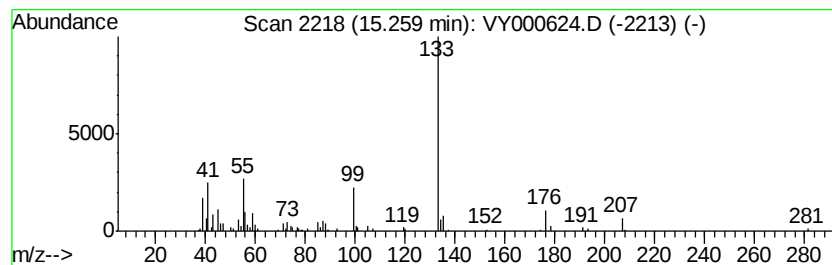
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Quant Title : SW846 8260

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

Peak Number 3 1,2,4-Triazole, 3,5-dithioxo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.26	21.21 ug/l	55349	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	58
2		(2-Methyl-[1,3]dithian-2-yl)phen...	240	C12H16OS2	078349-00-5	50
3		Rhodanine	133	C3H3NOS2	000141-84-4	47
4		1,3,4-Thiadiazole-2(3H)-thione, ...	133	C2H3N3S2	002349-67-9	28
5		(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	28



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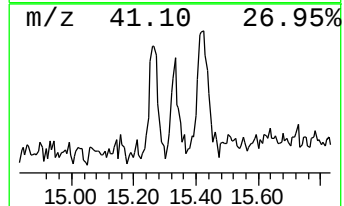
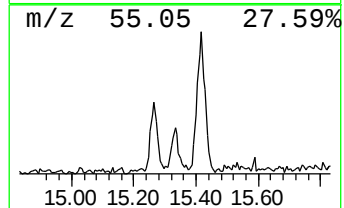
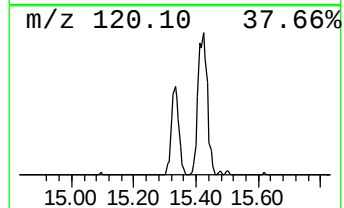
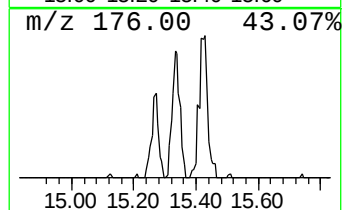
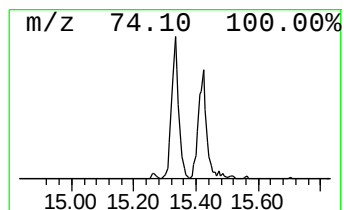
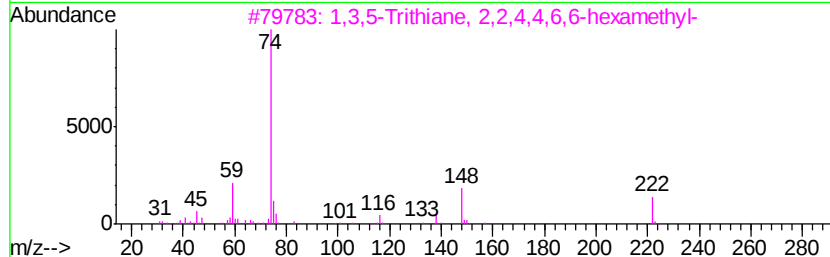
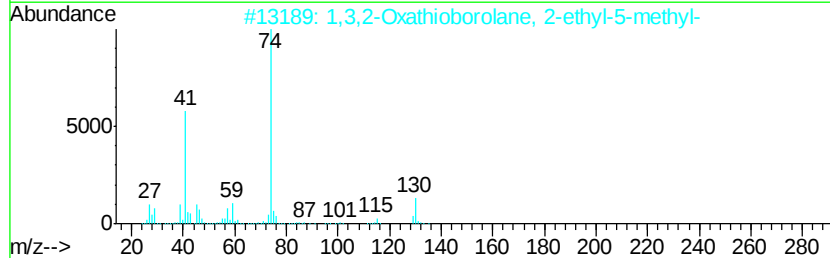
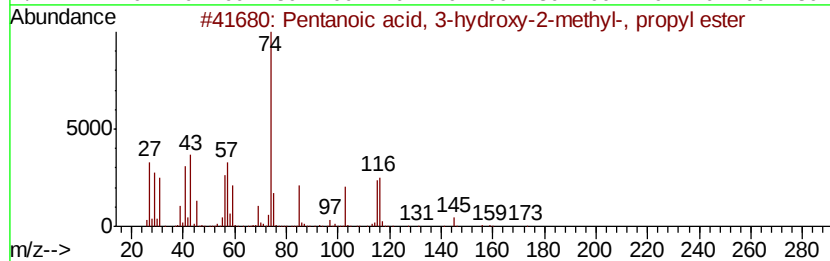
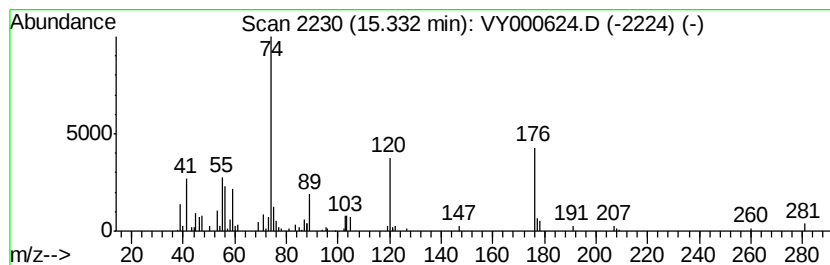
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown15.33 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.33	19.84 ug/l	51754	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 3-hydroxy-2-meth...	174	C9H18O3	1000151-17-3	38
2		1,3,2-Oxathioborolane, 2-ethyl-5...	130	C5H11BOS	1000163-05-5	35
3		1,3,5-Trithiane, 2,2,4,4,6,6-hex...	222	C9H18S3	000828-26-2	35
4		Propanoic acid	74	C3H6O2	000079-09-4	32
5		N,N-Dimethylformamide dipropyl a...	175	C9H21N02	006006-65-1	25



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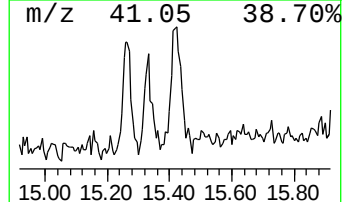
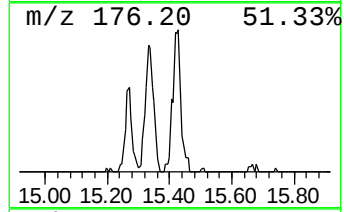
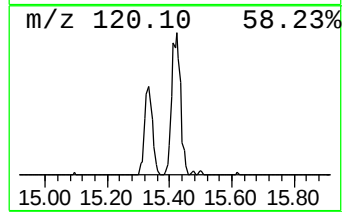
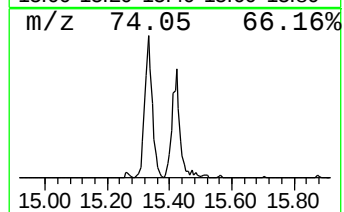
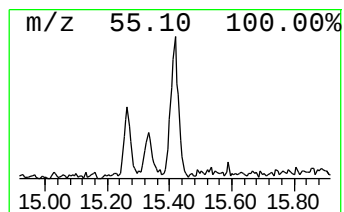
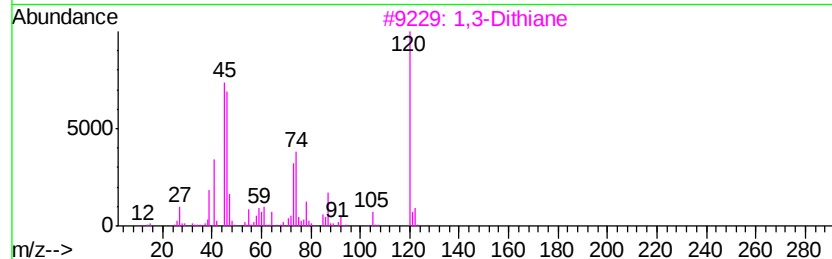
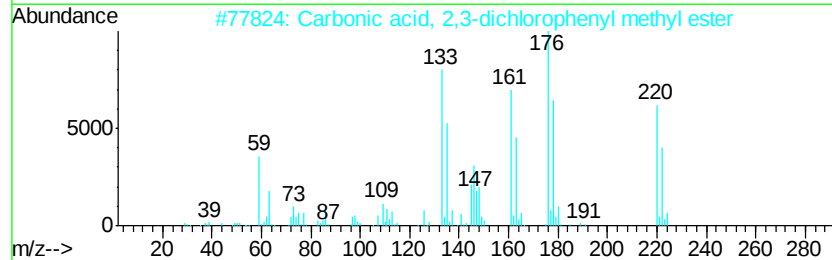
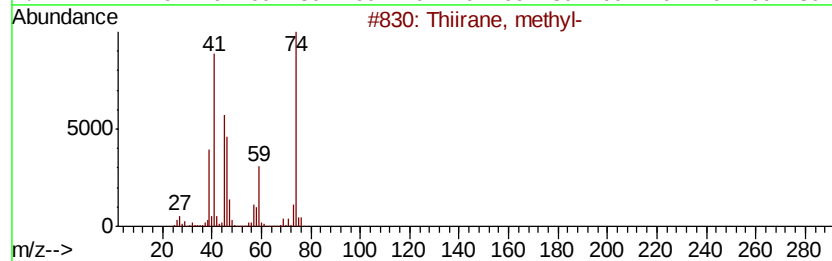
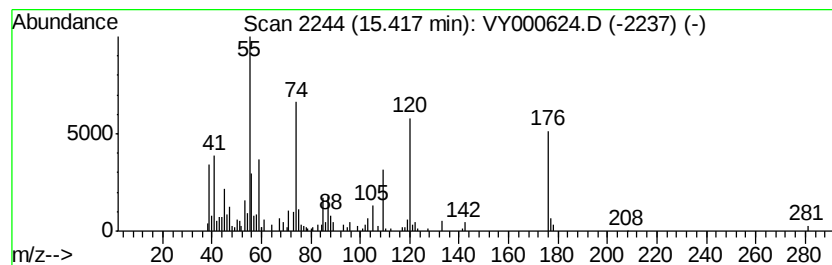
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Quant Title : SW846 8260

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

Peak Number 5 unknown15.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	35.91 ug/l	93678	1,4-Dichlorobenzene-d4	13.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiirane, methyl-	74	C3H6S	001072-43-1	25
2		Carbonic acid, 2,3-dichloropheny...	220	C8H6Cl2O3	1000331-47-7	18
3		1,3-Dithiane	120	C4H8S2	000505-23-7	14
4		Allyl mercaptan	74	C3H6S	000870-23-5	14
5		1,4-Dithiane	120	C4H8S2	000505-29-3	14



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY110819\
Data File : VY000624.D
Acq On : 08 Nov 2019 17:47
Operator : SY/MD
Sample : K5723-11
Misc : 7.08G/5ML/MSVOA Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
9-D

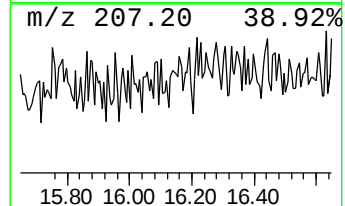
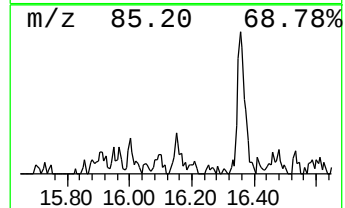
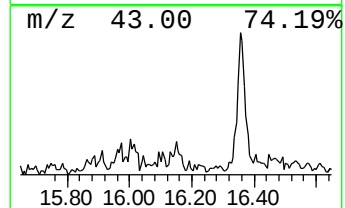
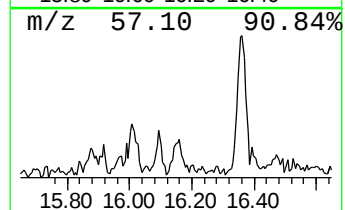
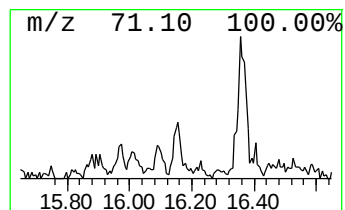
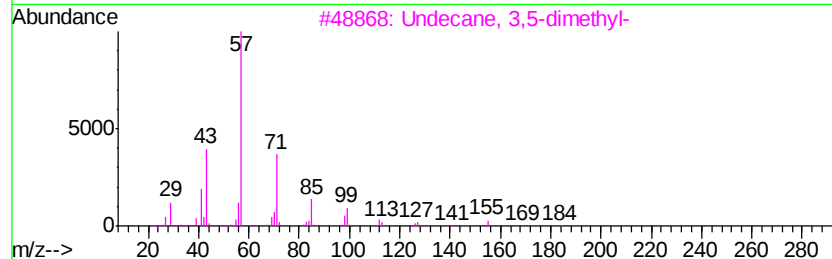
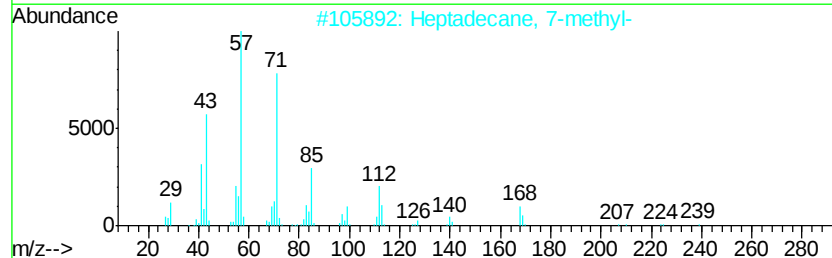
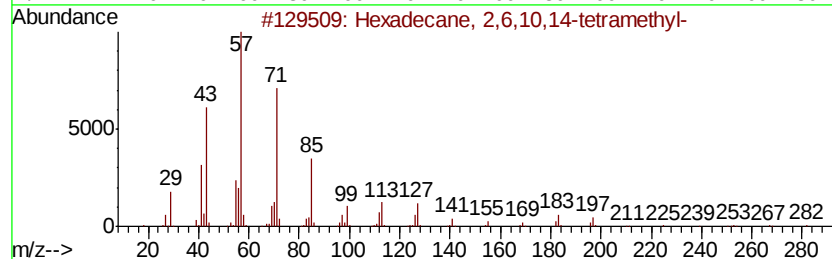
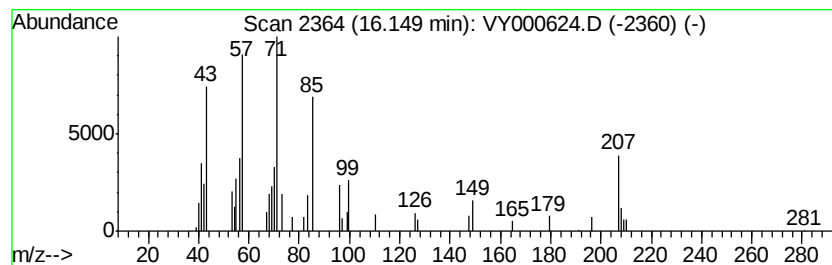
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Quant Title : SW846 8260

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

Peak Number 6 unknown16.15 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	5.62 ug/l	14671	1,4-Dichlorobenzene-d4	13.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	35
2	Heptadecane, 7-methyl-	254	C18H38	020959-33-5	35
3	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	35
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	35
5	Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA Y\DATA\VY110819\
Data File : VY000624.D
Acq On : 08 Nov 2019 17:47
Operator : SY/MD
Sample : K5723-11
Misc : 7.08G/5ML/MSVOA Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
9-D

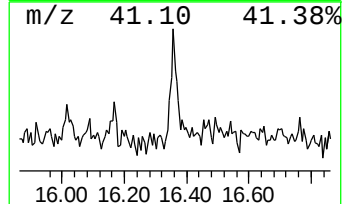
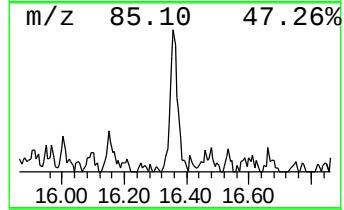
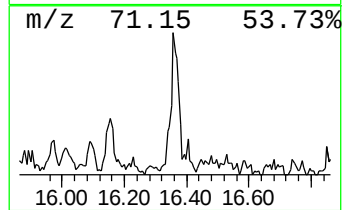
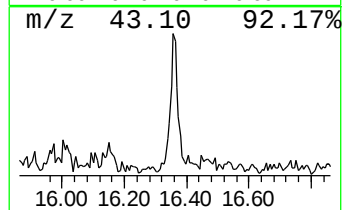
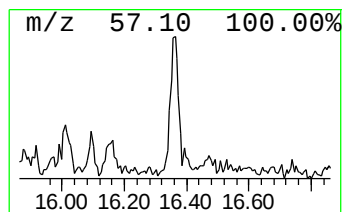
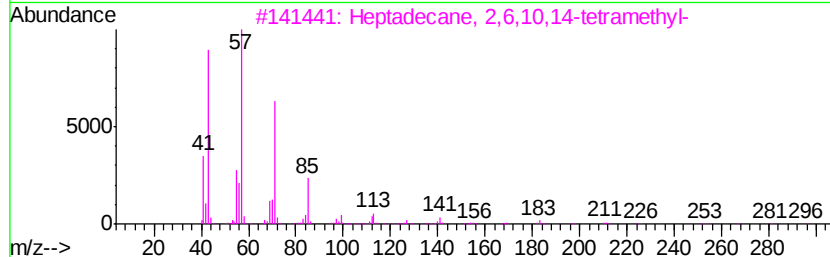
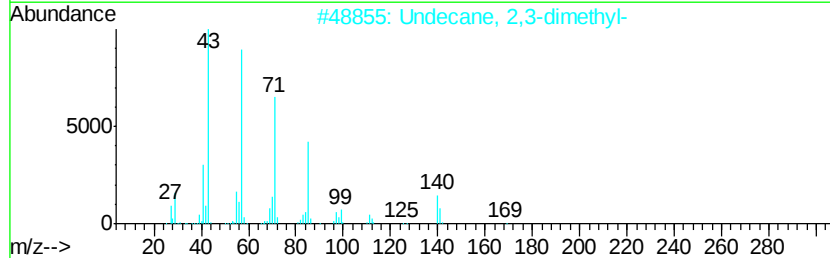
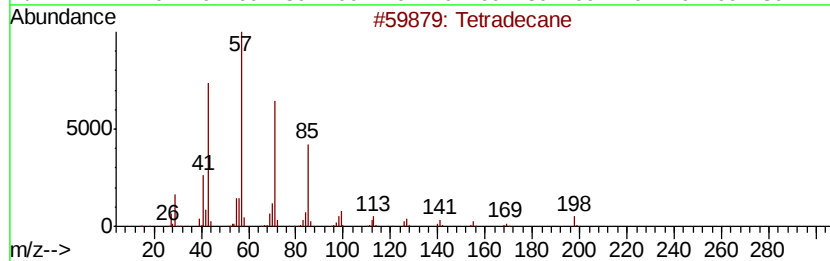
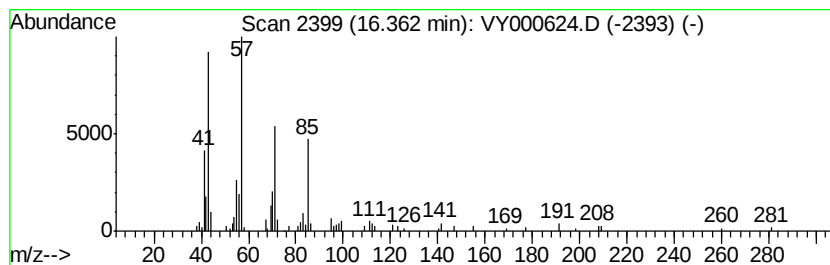
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Quant Title : SW846 8260

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

Peak Number 7 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	16.59 ug/l	43296	1,4-Dichlorobenzene-d4	13.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	76
2		Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	53
3		Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	50
4		Pentadecane	212	C15H32	000629-62-9	47
5		Undecane	156	C11H24	001120-21-4	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_Y\DATA\VY110819\
Data File : VY000624.D
Acq On : 08 Nov 2019 17:47
Operator : SY/MD
Sample : K5723-11
Misc : 7.08G/5ML/MSVOA_Y/SOIL
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
9-D

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_Y\METHODS\82Y103019S.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	5.75	5.2	ug/l	10216	1	7.80	99182	50.0
unknown13.30	13.30	5.0	ug/l	13126	4	13.42	130451	50.0
1,2,4-Triazole, 3...	15.26	21.2	ug/l	55349	4	13.42	130451	50.0
unknown15.33	15.33	19.8	ug/l	51754	4	13.42	130451	50.0
unknown15.42	15.42	35.9	ug/l	93678	4	13.42	130451	50.0
unknown16.15	16.15	5.6	ug/l	14671	4	13.42	130451	50.0
Tetradecane	16.36	16.6	ug/l	43296	4	13.42	130451	50.0