

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
 Data File : VY003927.D
 Acq On : 14 Jan 2021 18:24
 Operator : SY/MD
 Sample : M1141-20
 Misc : 5.02G/5ML/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 T872-T871

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_Y\methods\82Y011221S.M

Title : SW846 8260

Signal : TIC: VY003927.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.223	57	66	73	rBV2	9745	18929	1.57%	0.233%
2	4.716	465	475	487	rBV3	24974	77433	6.41%	0.951%
3	7.722	954	968	974	rBV	173198	413177	34.18%	5.076%
4	7.795	974	980	993	rVB	266369	603911	49.95%	7.420%
5	8.142	1026	1037	1050	rBV	182359	410692	33.97%	5.046%
6	8.691	1118	1127	1140	rBV	448701	878848	72.70%	10.798%
7	10.179	1362	1371	1379	rBV	712426	1208941	100.00%	14.854%
8	11.489	1576	1586	1593	rBV	618154	1006204	83.23%	12.363%
9	11.697	1614	1620	1626	rBV4	15588	31526	2.61%	0.387%
10	12.020	1668	1673	1679	rBV2	18796	31040	2.57%	0.381%
11	12.477	1738	1748	1759	rVB	462641	721591	59.69%	8.866%
12	12.764	1785	1795	1798	rBV2	55871	106131	8.78%	1.304%
13	12.806	1798	1802	1816	rVB4	20004	39466	3.26%	0.485%
14	12.965	1822	1828	1831	rBV6	7101	14560	1.20%	0.179%
15	13.038	1836	1840	1843	rVV	12123	19954	1.65%	0.245%
16	13.117	1847	1853	1857	rVB	24154	38651	3.20%	0.475%
17	13.166	1857	1861	1866	rBV4	8980	14088	1.17%	0.173%
18	13.282	1875	1880	1883	rBV4	17115	27316	2.26%	0.336%
19	13.361	1888	1893	1896	rVV4	26512	40458	3.35%	0.497%
20	13.422	1896	1903	1908	rVV	447887	709876	58.72%	8.722%
21	13.495	1908	1915	1917	rVV4	31367	80536	6.66%	0.989%
22	13.526	1917	1920	1928	rVB	44490	69291	5.73%	0.851%
23	13.751	1951	1957	1961	rBV	157747	241416	19.97%	2.966%
24	13.788	1961	1963	1968	rVB4	12940	21977	1.82%	0.270%
25	13.910	1978	1983	1988	rBV5	31373	52079	4.31%	0.640%
26	13.965	1988	1992	1996	rVB4	29413	42883	3.55%	0.527%
27	14.007	1996	1999	2005	rVB2	30125	52060	4.31%	0.640%
28	14.074	2005	2010	2014	rBV4	27741	42741	3.54%	0.525%
29	14.135	2014	2020	2026	rBV7	33223	72926	6.03%	0.896%
30	14.196	2026	2030	2032	rBV4	18834	28908	2.39%	0.355%
31	14.251	2033	2039	2040	rBV4	48253	78222	6.47%	0.961%
32	14.312	2046	2049	2055	rVB4	34592	56957	4.71%	0.700%
33	14.379	2056	2060	2063	rBV4	51876	76393	6.32%	0.939%
34	14.416	2063	2066	2070	rVB5	33161	44173	3.65%	0.543%
35	14.605	2094	2097	2103	rVB	90847	122819	10.16%	1.509%
36	14.678	2103	2109	2113	rBV7	33328	73714	6.10%	0.906%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
T872-T871

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_Y\methods\82Y011221S.M
Title : SW846 8260

37	14.727	2113	2117	2123	rVB2	53186	89012	7.36%	1.094%
38	14.842	2133	2136	2138	rBV4	15167	20432	1.69%	0.251%
39	14.867	2138	2140	2145	rVB6	23794	34718	2.87%	0.427%
40	14.940	2148	2152	2156	rVB5	25164	34747	2.87%	0.427%
41	15.001	2156	2162	2173	rBV	166153	330840	27.37%	4.065%
42	15.428	2229	2232	2238	rVB4	34629	59447	4.92%	0.730%

Sum of corrected areas: 8139083

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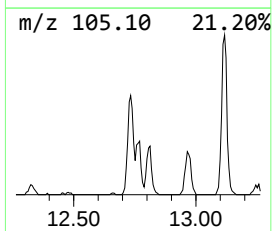
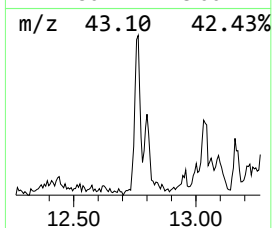
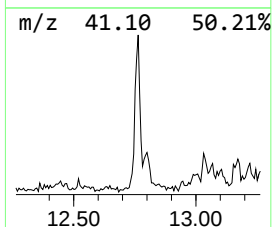
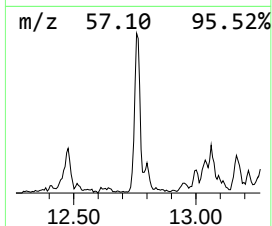
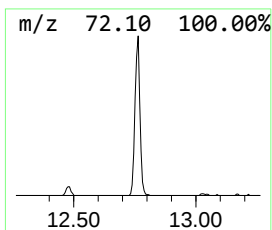
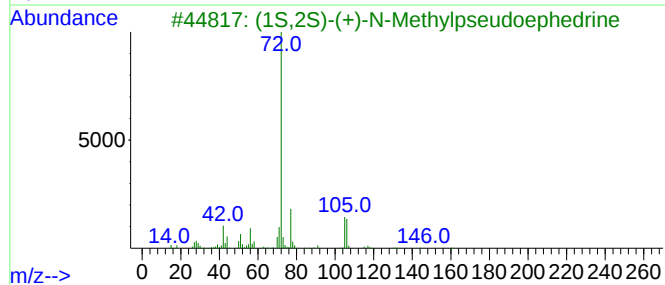
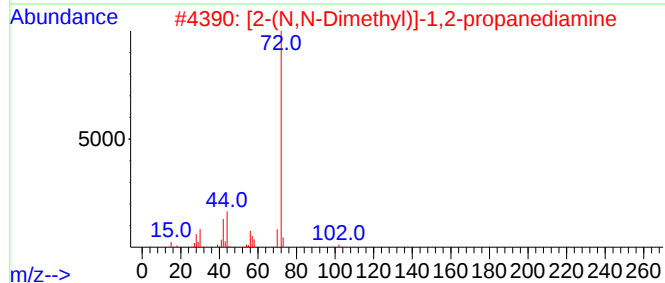
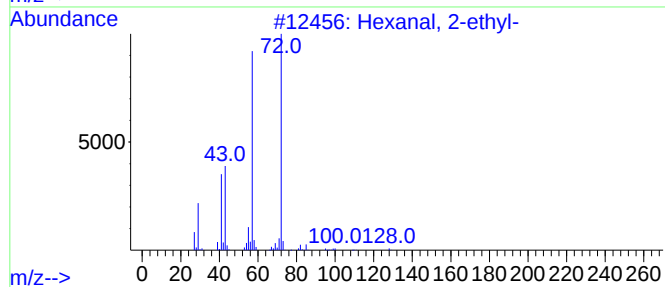
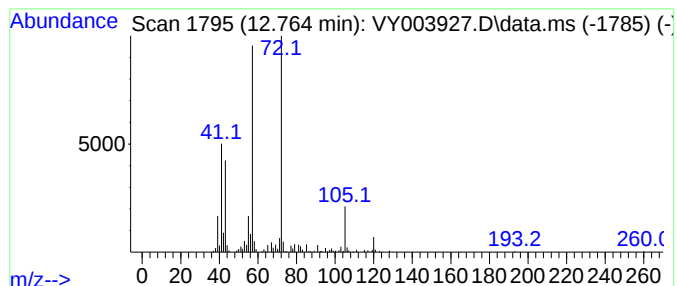
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Quant Title : SW846 8260

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

Peak Number 1 Hexanal, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.764	7.48 ug/l	106131	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	70
2			[2-(N,N-Dimethyl)]-1,2-propanedi...	102	C5H14N2	1000133-38-7	50
3			(1S,2S)-(+)-N-Methylpseudoephedrine	179	C11H17NO	051018-28-1	50
4			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	42
5			Methylpseudoephedrine -	179	C11H17NO	1000334-93-4	40



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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

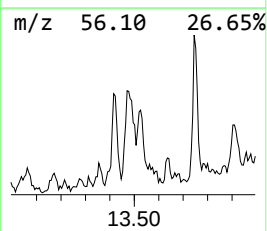
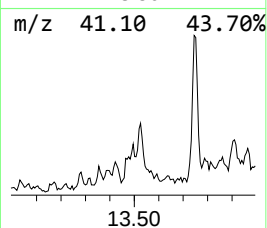
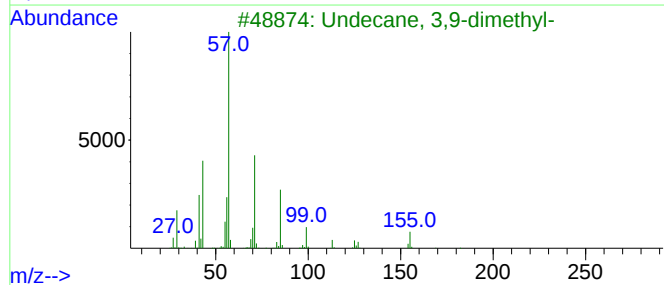
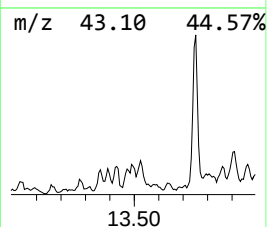
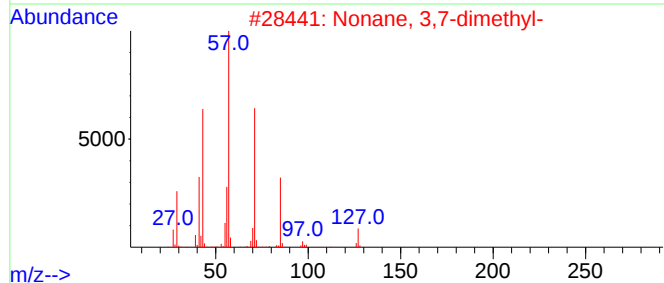
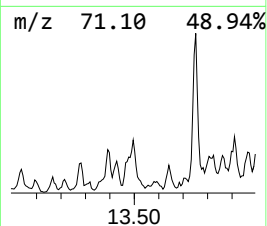
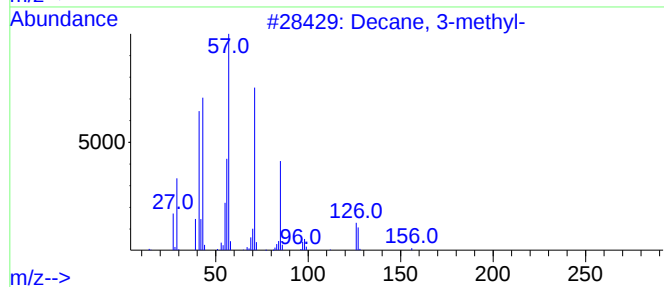
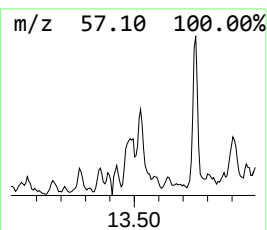
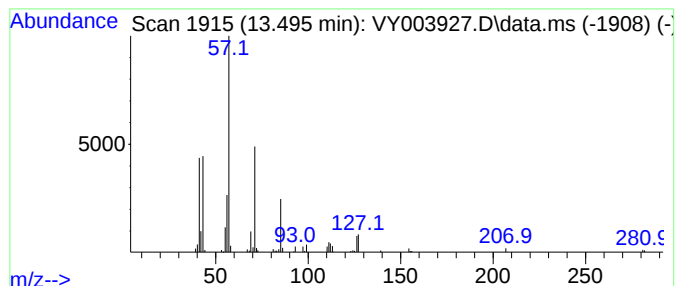
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Quant Title : SW846 8260

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

Peak Number 2 Decane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.495	5.67 ug/l	80536	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 3-methyl-	156	C11H24	013151-34-3	74
2			Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
3			Undecane, 3,9-dimethyl-	184	C13H28	017301-31-4	64
4			Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	64
5			Nonane, 3-methyl-5-propyl-	184	C13H28	031081-18-2	59



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Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

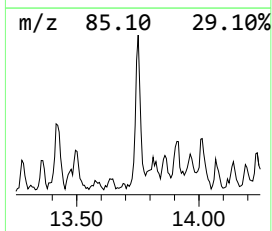
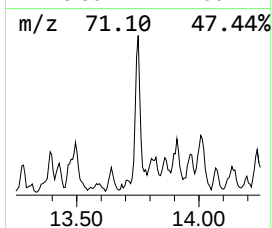
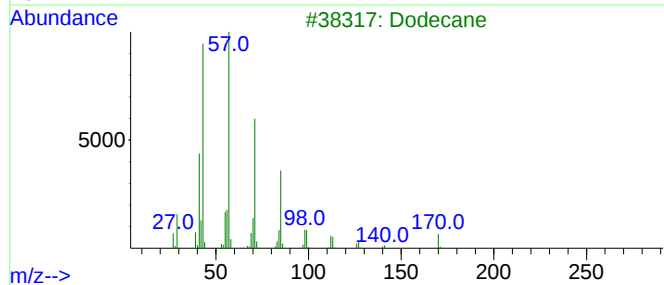
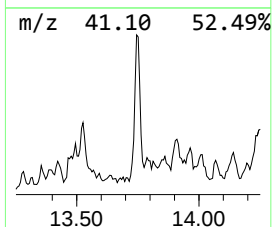
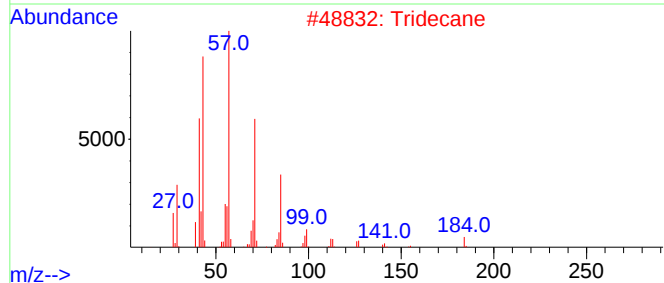
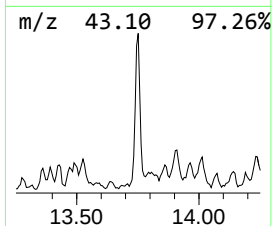
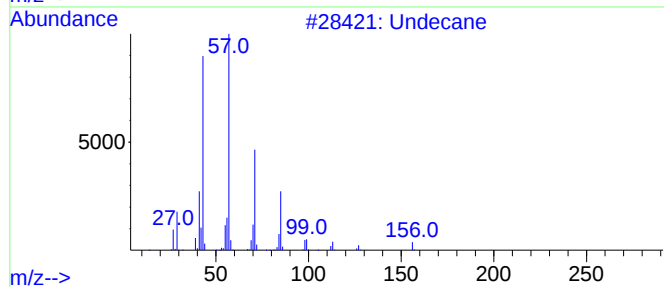
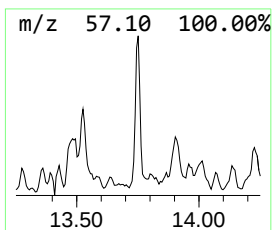
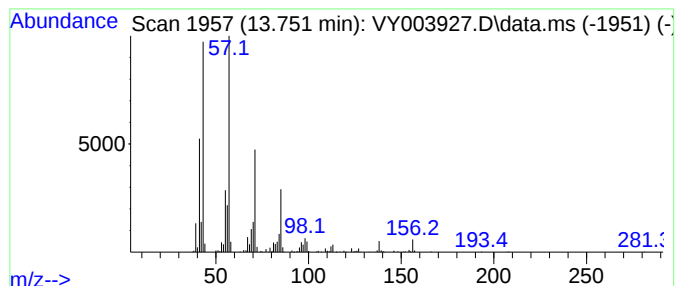
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.M
Quant Title : SW846 8260

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

Peak Number 3 Undecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.751	17.00 ug/l	241416	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	93
2	Tridecane			184	C13H28	000629-50-5	80
3	Dodecane			170	C12H26	000112-40-3	80
4	Pentadecane			212	C15H32	000629-62-9	72
5	Hexadecane			226	C16H34	000544-76-3	64



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Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

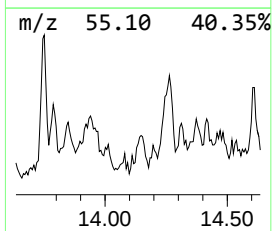
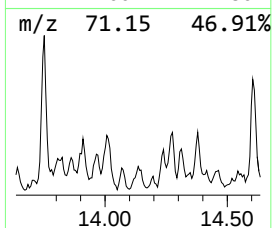
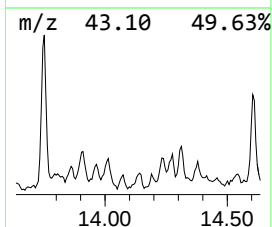
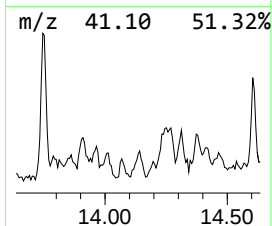
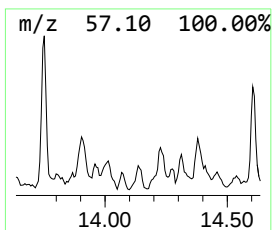
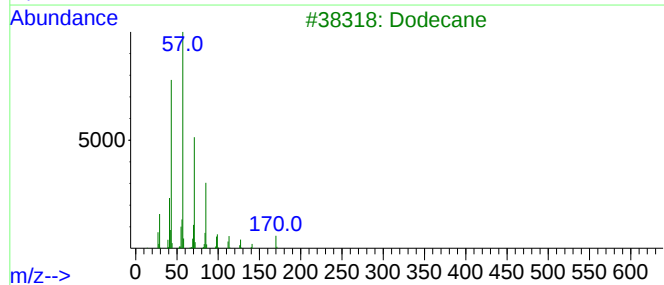
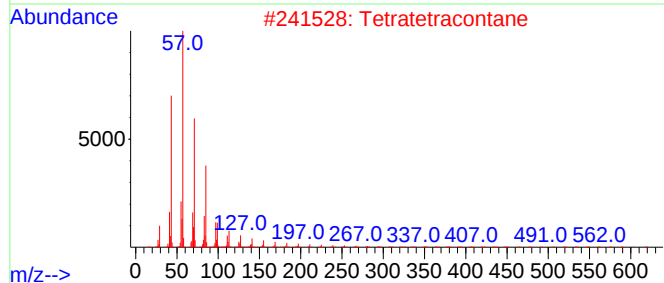
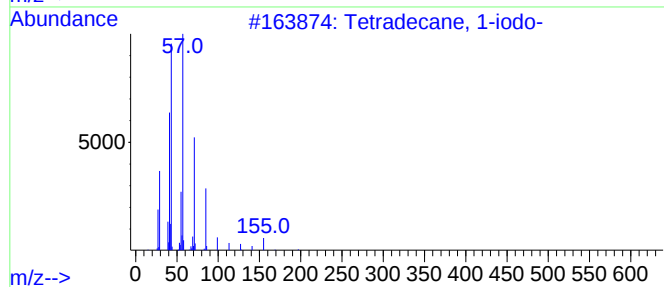
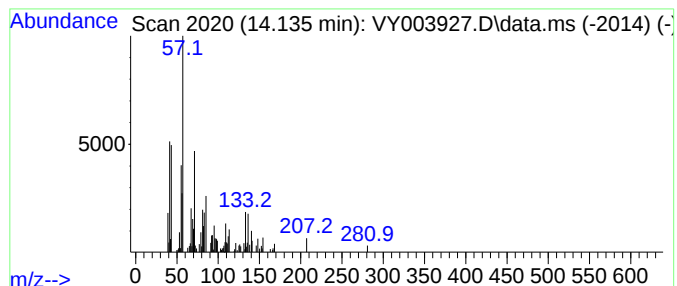
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown14.135 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.135	5.14 ug/l	72926	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	38
2			Tetratetracontane	619	C44H90	007098-22-8	38
3			Dodecane	170	C12H26	000112-40-3	38
4			Tridecane	184	C13H28	000629-50-5	38
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	38



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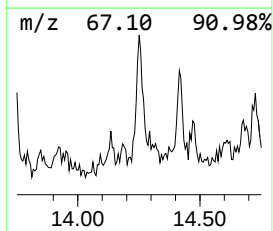
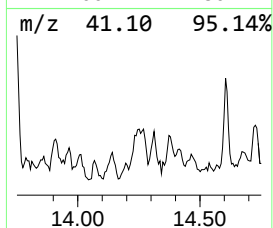
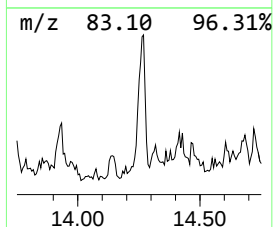
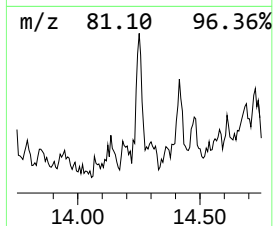
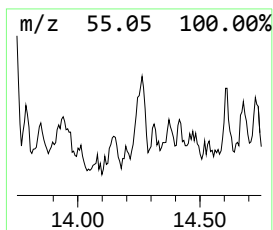
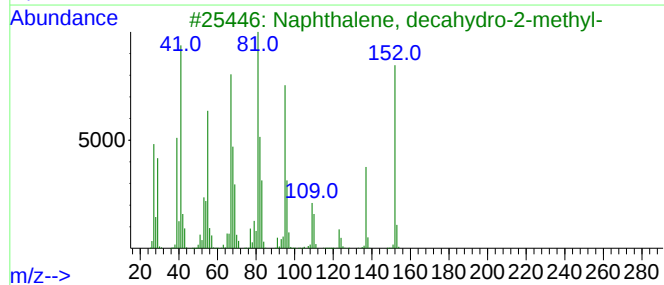
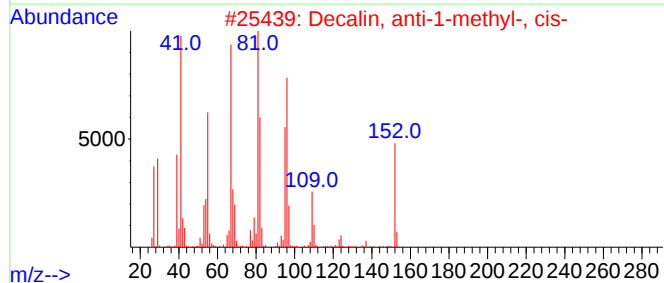
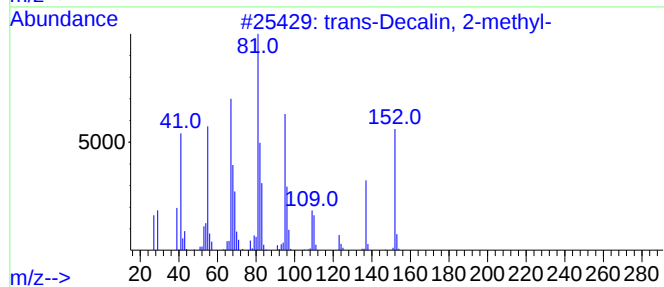
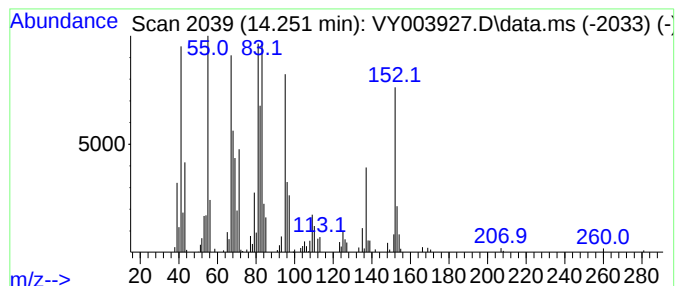
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.M
Quant Title : SW846 8260

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

Peak Number 5 trans-Decalin, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	5.51 ug/l	78222	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	81
2			Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	64
3			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	60
4			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	58
5			Bicyclo[4.1.0]heptan-3-one, 4,7,...	152	C10H16O	004176-04-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
Data File : VY003927.D
Acq On : 14 Jan 2021 18:24
Operator : SY/MD
Sample : M1141-20
Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

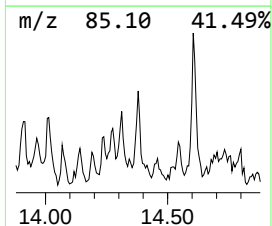
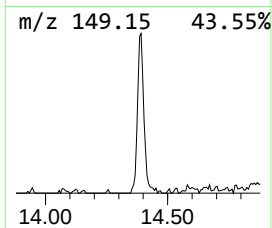
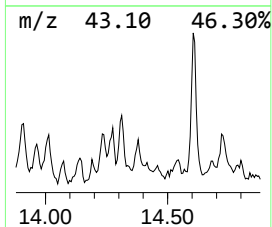
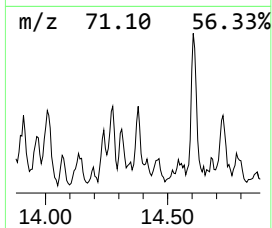
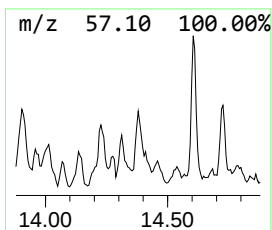
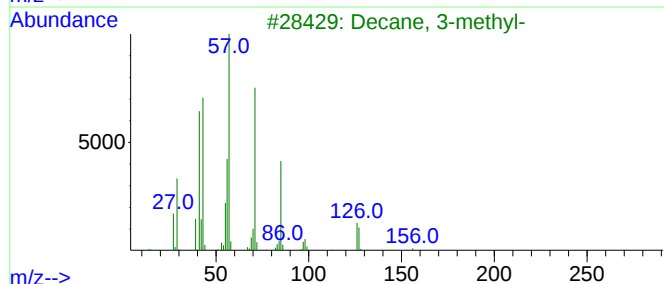
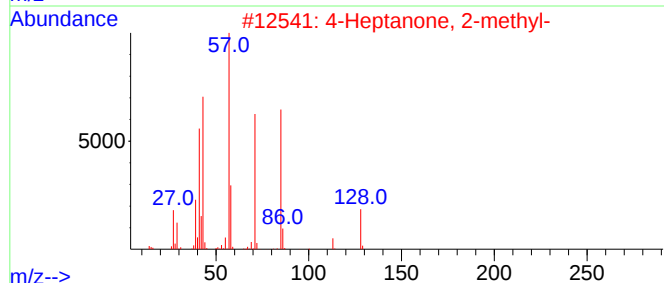
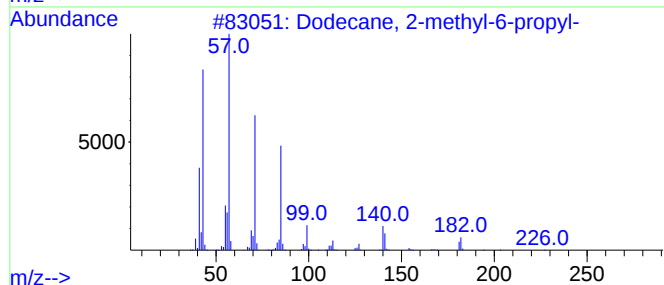
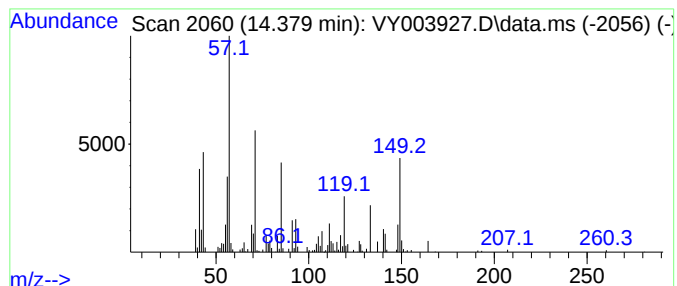
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.379 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.379	5.38 ug/l	76393	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	38
2			4-Heptanone, 2-methyl-	128	C8H16O	000626-33-5	35
3			Decane, 3-methyl-	156	C11H24	013151-34-3	35
4			Tridecane, 3-methyl-	198	C14H30	006418-41-3	35
5			Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
Data File : VY003927.D
Acq On : 14 Jan 2021 18:24
Operator : SY/MD
Sample : M1141-20
Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

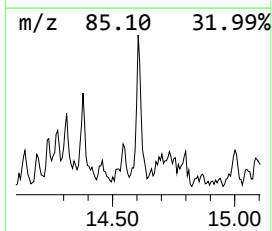
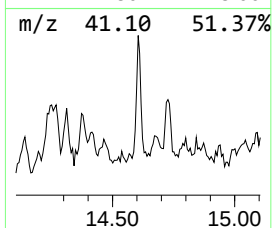
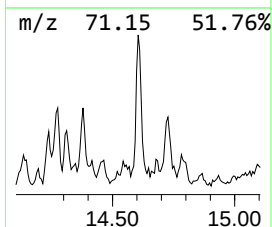
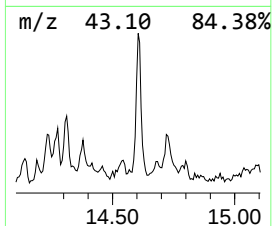
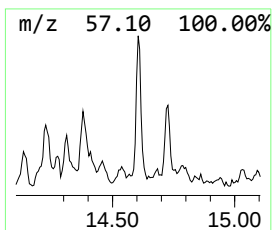
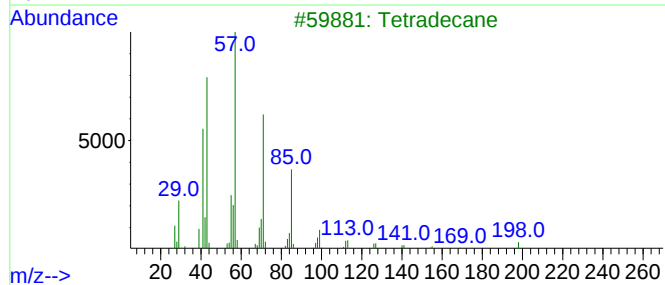
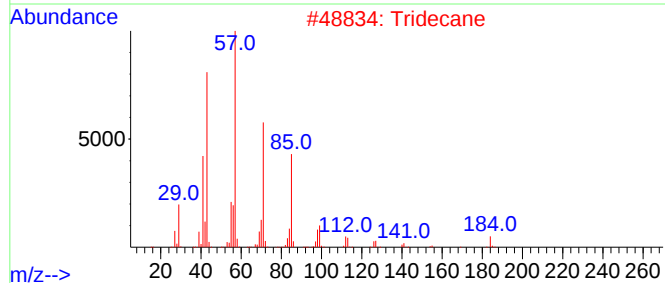
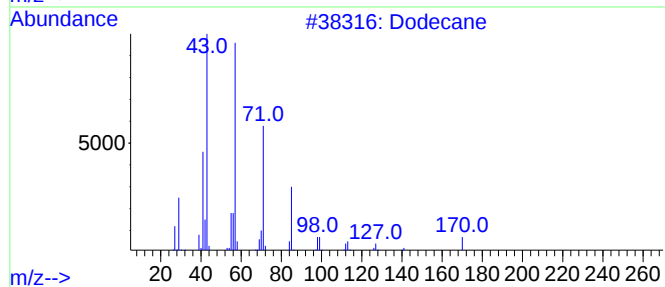
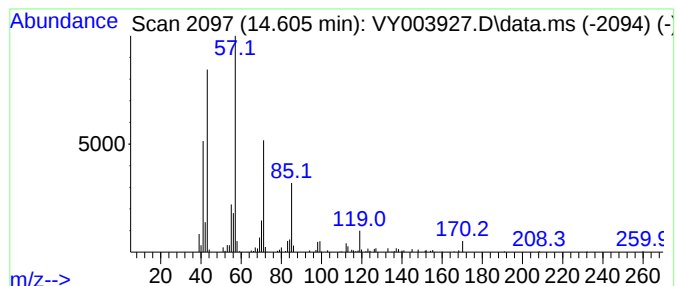
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Quant Title : SW846 8260

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

Peak Number 7 Dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.605	8.65 ug/l	122819	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	91
2			Tridecane	184	C13H28	000629-50-5	80
3			Tetradecane	198	C14H30	000629-59-4	80
4			Hexadecane	226	C16H34	000544-76-3	64
5			Nonadecane, 2-methyl-	282	C20H42	001560-86-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
Data File : VY003927.D
Acq On : 14 Jan 2021 18:24
Operator : SY/MD
Sample : M1141-20
Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

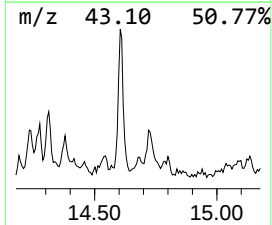
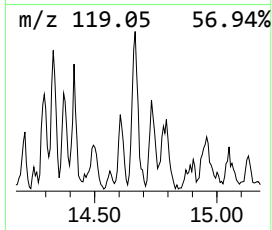
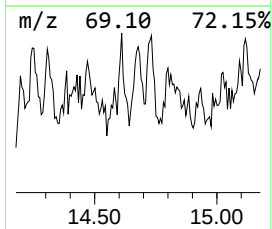
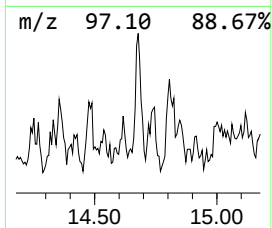
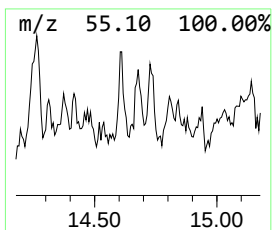
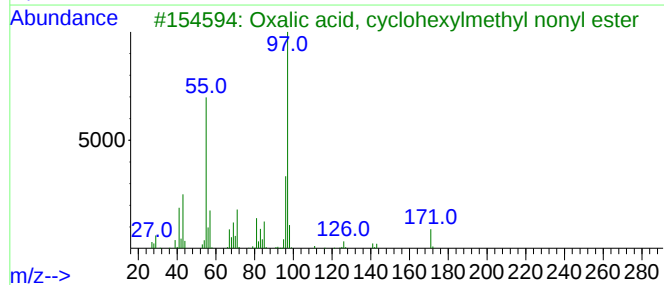
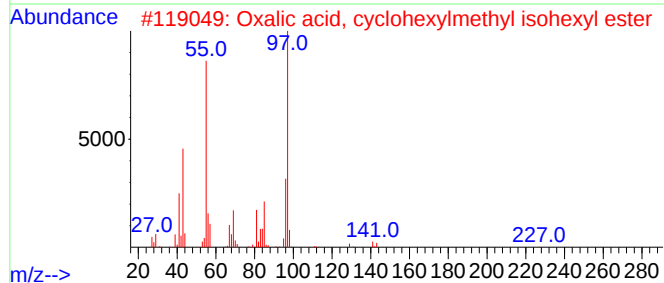
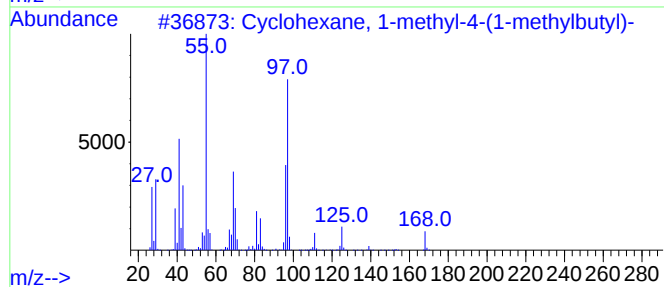
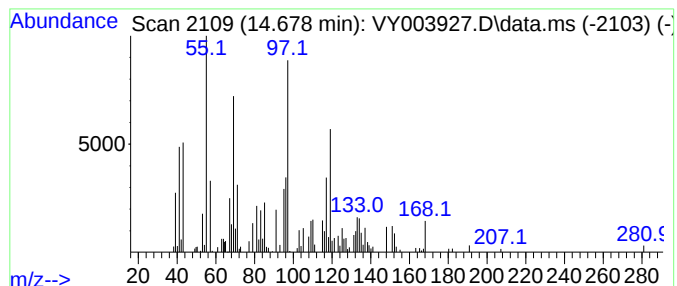
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.M
Quant Title : SW846 8260

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

Peak Number 8 unknown14.678 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.678	5.19 ug/l	73714	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-methyl-4-(1-methy...	168	C12H24	054411-00-6	38
2			Oxalic acid, cyclohexylmethyl is...	270	C15H26O4	1000309-68-3	38
3			Oxalic acid, cyclohexylmethyl no...	312	C18H32O4	1000309-68-6	35
4			Oxalic acid, cyclohexylmethyl de...	326	C19H34O4	1000309-68-7	35
5			Oxalic acid, cyclohexylmethyl tr...	368	C22H40O4	1000309-69-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
Data File : VY003927.D
Acq On : 14 Jan 2021 18:24
Operator : SY/MD
Sample : M1141-20
Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

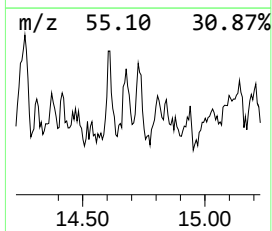
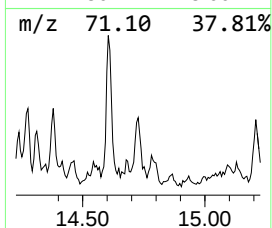
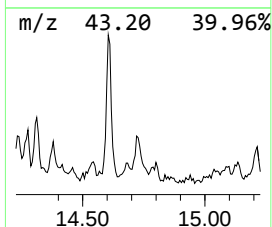
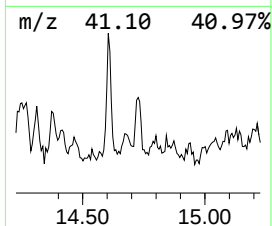
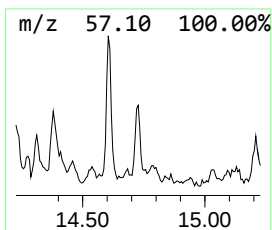
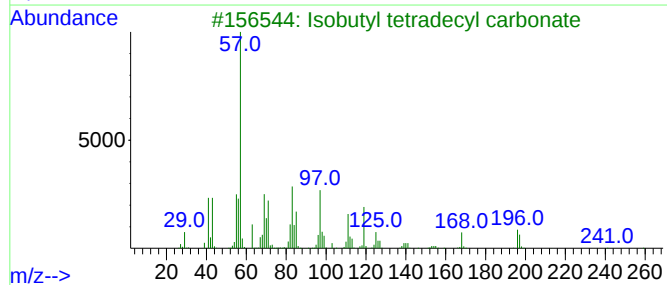
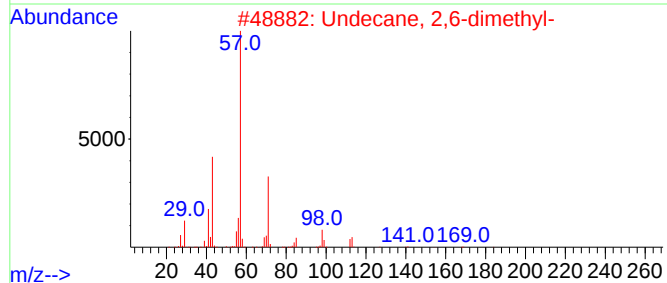
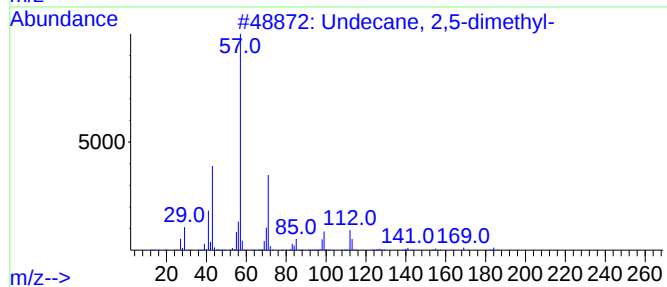
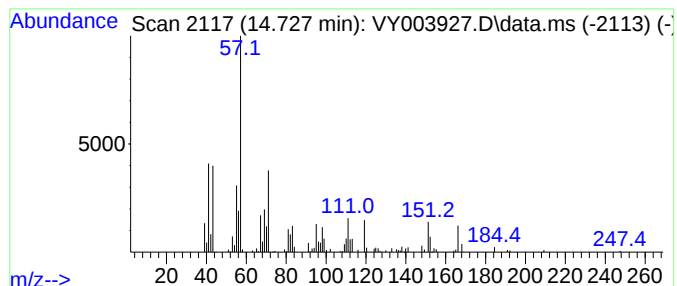
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown14.727 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.727	6.27 ug/l	89012	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	46
2			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	43
3			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	40
4			Carbonic acid, isobutyl pentadec...	328	C20H40O3	1000314-61-2	40
5			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY011421\
Data File : VY003927.D
Acq On : 14 Jan 2021 18:24
Operator : SY/MD
Sample : M1141-20
Misc : 5.02G/5ML/MSVOA_Y/SOIL
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
T872-T871

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y011221S.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
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Decane, 3-methyl-	13.495	5.7	ug/l	80536	4	13.422	709876	50.0
Undecane	13.751	17.0	ug/l	241416	4	13.422	709876	50.0
unknown14.135	14.135	5.1	ug/l	72926	4	13.422	709876	50.0
trans-Decalin, ...	14.251	5.5	ug/l	78222	4	13.422	709876	50.0
unknown14.379	14.379	5.4	ug/l	76393	4	13.422	709876	50.0
Dodecane	14.605	8.7	ug/l	122819	4	13.422	709876	50.0
unknown14.678	14.678	5.2	ug/l	73714	4	13.422	709876	50.0
unknown14.727	14.727	6.3	ug/l	89012	4	13.422	709876	50.0