

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111821\
 Data File : VY006816.D
 Acq On : 18 Nov 2021 18:55
 Operator : SY/MD
 Sample : M4762-05
 Misc : 4.99G/5ML/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 COMP-1-3

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\82Y111521S.M
 Title : SW846 8260

Signal : TIC: VY006816.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.723	147	148	151	rBV2	323	323	6.72%	0.553%
2	2.796	157	160	164	rBV4	300	480	9.99%	0.822%
3	2.893	173	176	177	rVB3	280	247	5.14%	0.423%
4	2.905	177	178	180	rBV	278	205	4.27%	0.351%
5	2.979	188	190	193	rBV3	178	248	5.16%	0.425%
6	3.009	193	195	198	rVB2	339	311	6.47%	0.532%
7	3.058	198	203	204	rBV3	208	236	4.91%	0.404%
8	3.235	229	232	234	rBV	178	202	4.20%	0.346%
9	3.430	261	264	267	rVB3	191	209	4.35%	0.358%
10	3.466	267	270	272	rBV	155	214	4.45%	0.366%
11	3.485	272	273	279	rVB2	163	204	4.24%	0.349%
12	3.863	332	335	336	rBV2	226	233	4.85%	0.399%
13	3.936	343	347	349	rBV2	286	372	7.74%	0.637%
14	4.131	375	379	380	rVV2	236	285	5.93%	0.488%
15	4.722	469	476	478	rBV	385	368	7.66%	0.630%
16	5.216	553	557	560	rVB2	146	202	4.20%	0.346%
17	5.295	568	570	574	rVB2	179	209	4.35%	0.358%
18	5.374	581	583	585	rVB	259	225	4.68%	0.385%
19	5.429	589	592	595	rVB2	209	216	4.49%	0.370%
20	5.545	606	611	613	rVB2	191	223	4.64%	0.382%
21	5.783	647	650	651	rBV2	285	246	5.12%	0.421%
22	5.826	654	657	660	rBV	172	265	5.51%	0.454%
23	5.911	670	671	674	rVB	286	226	4.70%	0.387%
24	5.941	674	676	682	rBV2	271	419	8.72%	0.717%
25	6.063	692	696	697	rBV2	202	273	5.68%	0.467%
26	6.265	726	729	731	rBV	204	234	4.87%	0.401%
27	6.386	747	749	752	rBV2	226	321	6.68%	0.550%
28	6.490	763	766	767	rBV2	199	205	4.27%	0.351%
29	6.746	806	808	809	rBV	211	225	4.68%	0.385%
30	6.832	821	822	826	rBV3	180	236	4.91%	0.404%
31	6.947	839	841	844	rVB2	247	226	4.70%	0.387%
32	7.051	857	858	861	rVB2	279	244	5.08%	0.418%
33	7.081	861	863	866	rBV2	252	376	7.82%	0.644%
34	7.210	879	884	888	rBV2	146	212	4.41%	0.363%
35	7.466	924	926	928	rBV3	201	248	5.16%	0.425%
36	7.496	930	931	933	rBV2	384	329	6.85%	0.563%

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37	7.527	933	936	938	rVV2	348	460	9.57%	0.788%
38	7.618	948	951	953	rBV2	261	322	6.70%	0.551%
39	7.703	963	965	966	rBV	238	245	5.10%	0.419%
40	7.716	966	967	972	rVV4	615	853	17.75%	1.460%
41	7.789	977	979	986	rVB3	717	1423	29.61%	2.436%
42	8.039	1017	1020	1023	rVB2	282	260	5.41%	0.445%
43	8.081	1023	1027	1029	rVB3	151	217	4.52%	0.372%
44	8.106	1029	1031	1033	rBV	225	210	4.37%	0.360%
45	8.142	1033	1037	1042	rBV3	1118	2182	45.40%	3.736%
46	8.325	1064	1067	1068	rBV2	166	227	4.72%	0.389%
47	8.380	1073	1076	1077	rBV	185	213	4.43%	0.365%
48	8.557	1104	1105	1108	rVB2	264	248	5.16%	0.425%
49	8.691	1124	1127	1133	rVB3	1579	2588	53.85%	4.431%
50	9.447	1248	1251	1254	rVB2	185	212	4.41%	0.363%
51	9.703	1288	1293	1295	rBV2	152	267	5.56%	0.457%
52	10.185	1367	1372	1378	rVB2	2701	4503	93.70%	7.710%
53	10.575	1435	1436	1438	rBV	222	211	4.39%	0.361%
54	10.819	1472	1476	1479	rVB2	280	376	7.82%	0.644%
55	10.849	1479	1481	1485	rBV2	252	362	7.53%	0.620%
56	11.014	1506	1508	1510	rBV	260	247	5.14%	0.423%
57	11.239	1540	1545	1546	rBV2	392	427	8.88%	0.731%
58	11.264	1546	1549	1550	rVB2	356	363	7.55%	0.622%
59	11.349	1559	1563	1567	rBV3	402	477	9.93%	0.817%
60	11.416	1569	1574	1575	rBV3	333	472	9.82%	0.808%
61	11.495	1582	1587	1591	rBV3	2852	4238	88.18%	7.256%
62	11.532	1591	1593	1594	rVV2	475	299	6.22%	0.512%
63	11.550	1594	1596	1598	rVV2	350	237	4.93%	0.406%
64	11.575	1598	1600	1604	rVV3	383	493	10.26%	0.844%
65	11.629	1607	1609	1611	rVB3	413	347	7.22%	0.594%
66	11.709	1619	1622	1623	rBV	348	271	5.64%	0.464%
67	11.721	1623	1624	1627	rVB2	293	253	5.26%	0.433%
68	11.806	1637	1638	1640	rBV	307	247	5.14%	0.423%
69	11.831	1640	1642	1646	rVV2	393	514	10.69%	0.880%
70	11.873	1646	1649	1651	rVV2	369	445	9.26%	0.762%
71	11.898	1651	1653	1654	rVB	571	291	6.05%	0.498%
72	11.940	1658	1660	1663	rBV3	295	383	7.97%	0.656%
73	12.026	1672	1674	1676	rBV2	293	379	7.89%	0.649%
74	12.087	1679	1684	1685	rBV5	466	605	12.59%	1.036%
75	12.105	1685	1687	1688	rBV2	746	706	14.69%	1.209%
76	12.221	1704	1706	1709	rVV3	649	479	9.97%	0.820%

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77	12.373	1729	1731	1735	rBV2	436	540	11.24%	0.925%
78	12.495	1744	1751	1755	rBV8	2351	4806	100.00%	8.229%
79	12.617	1770	1771	1773	rVB2	540	374	7.78%	0.640%
80	12.769	1792	1796	1798	rBV4	425	548	11.40%	0.938%
81	12.873	1811	1813	1817	rVB4	654	891	18.54%	1.526%
82	12.910	1817	1819	1820	rBV2	486	383	7.97%	0.656%
83	13.068	1843	1845	1846	rBV2	448	203	4.22%	0.348%
84	13.202	1865	1867	1868	rBV2	769	661	13.75%	1.132%
85	13.422	1898	1903	1910	rVB9	1822	4057	84.42%	6.946%
86	13.861	1973	1975	1978	rBV4	809	926	19.27%	1.585%
87	13.928	1984	1986	1987	rBV2	703	563	11.71%	0.964%
88	14.379	2058	2060	2062	rBV3	740	573	11.92%	0.981%
89	14.434	2067	2069	2072	rVB2	623	627	13.05%	1.074%
90	14.580	2090	2093	2094	rBV3	659	790	16.44%	1.353%
91	15.056	2169	2171	2172	rBV2	557	354	7.37%	0.606%
92	15.287	2207	2209	2212	rBV3	562	495	10.30%	0.848%
93	15.440	2232	2234	2235	rVB2	510	323	6.72%	0.553%
94	15.507	2241	2245	2248	rBV6	857	1291	26.86%	2.210%
95	15.592	2257	2259	2261	rVB3	501	284	5.91%	0.486%
96	15.897	2307	2309	2312	rBV3	438	577	12.01%	0.988%
97	16.007	2325	2327	2328	rVB	538	306	6.37%	0.524%
98	16.037	2330	2332	2336	rBV3	528	487	10.13%	0.834%
99	16.244	2364	2366	2368	rBV2	458	450	9.36%	0.770%
100	16.629	2427	2429	2432	rBV4	662	847	17.62%	1.450%

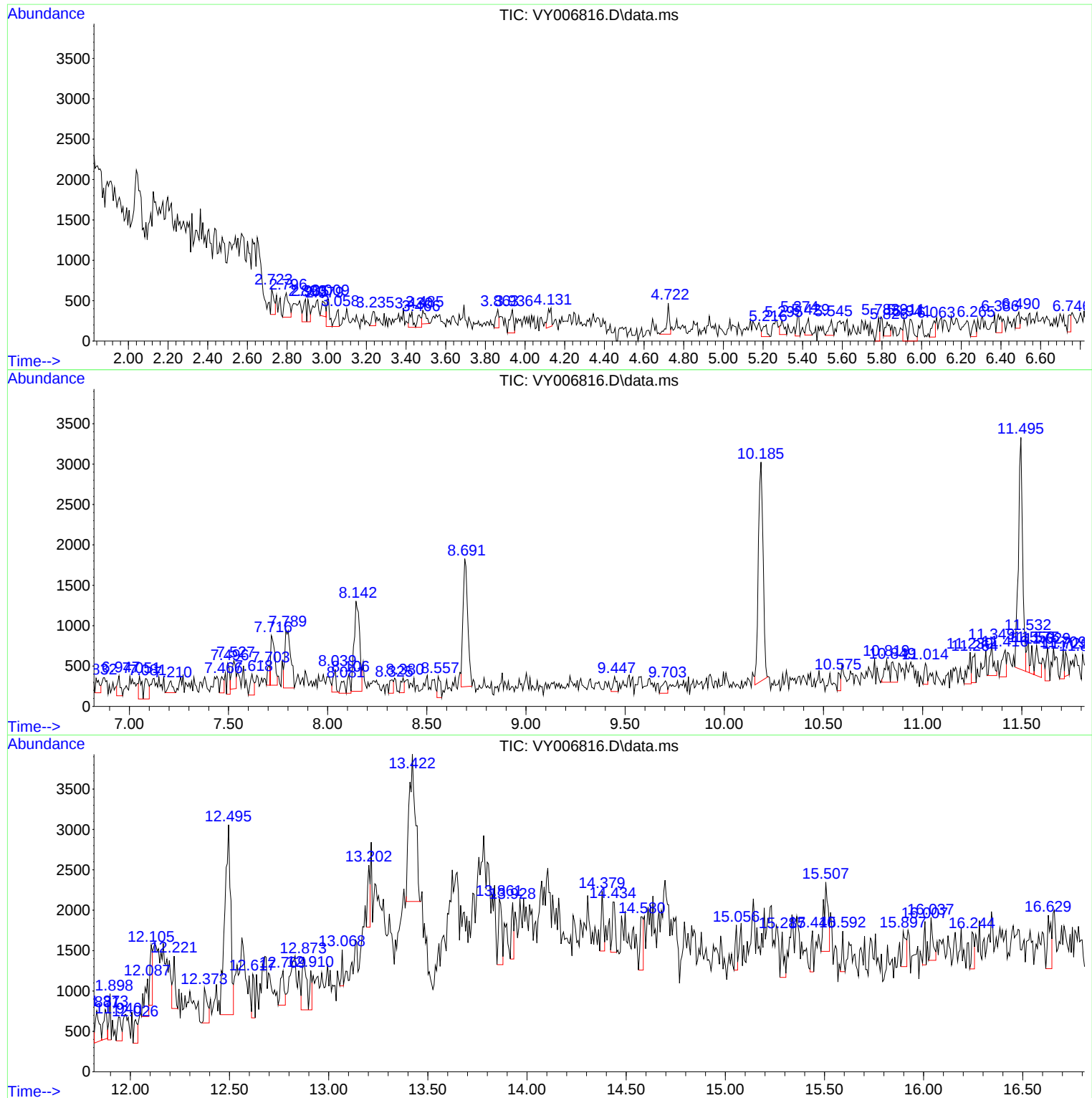
Sum of corrected areas: 58405

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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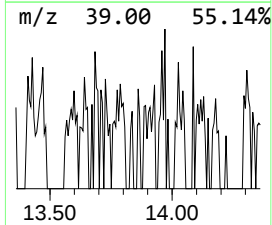
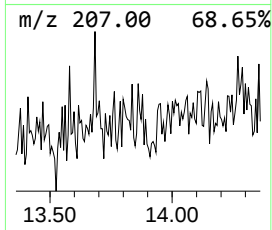
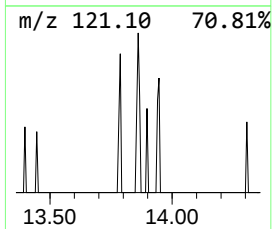
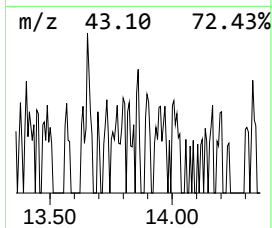
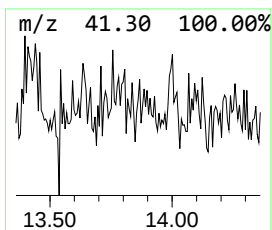
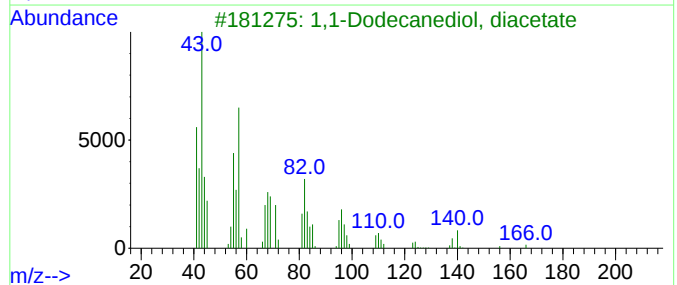
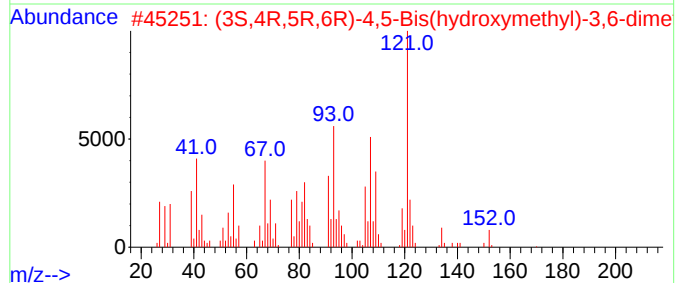
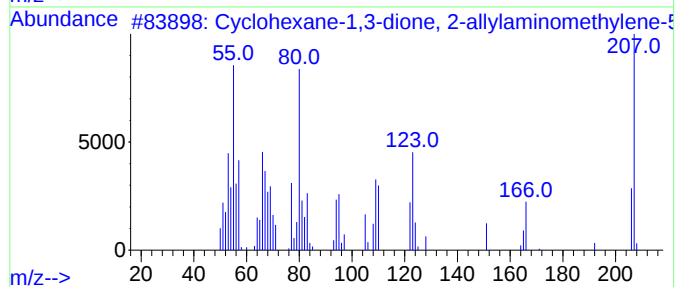
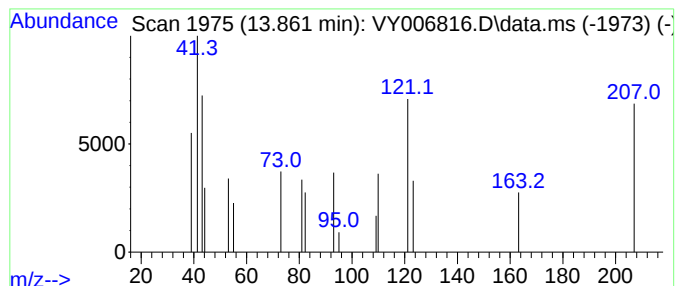
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown13.861 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.861	11.41 ug/l	926	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	12
2			(3S,4R,5R,6R)-4,5-Bis(hydroxymet...	170	C10H18O2	1000099-24-3	9
3			1,1-Dodecanediol, diacetate	286	C16H30O4	056438-07-4	9
4			Cyclohexanol, 3-(aminomethyl)-3,...	171	C10H21NO	015647-11-7	9
5			6-Octenoic acid, 3,7-dimethyl-, ...	184	C11H20O2	002270-60-2	9



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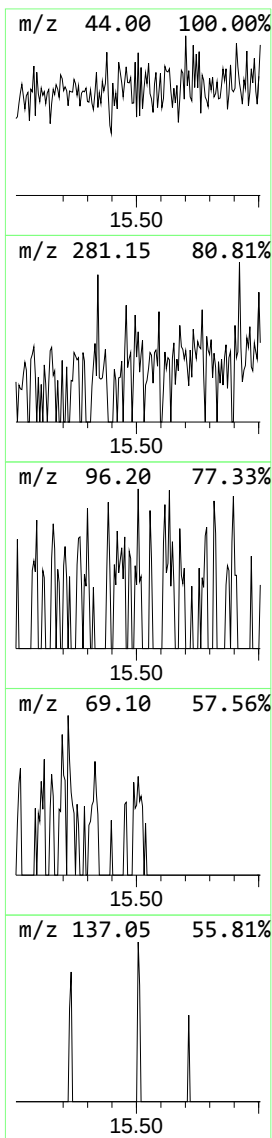
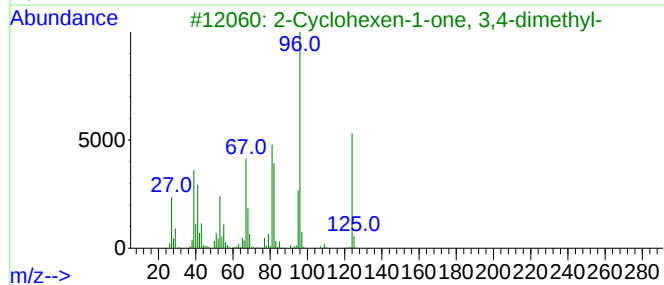
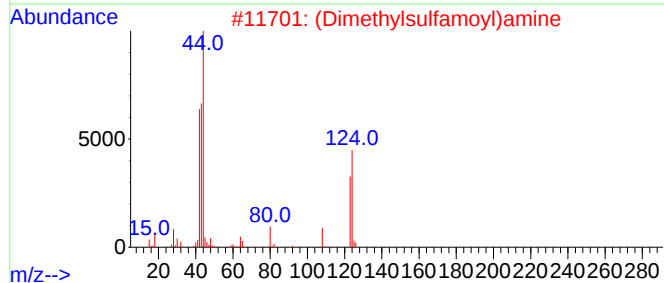
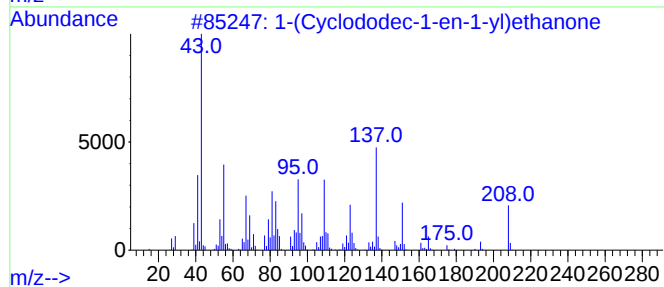
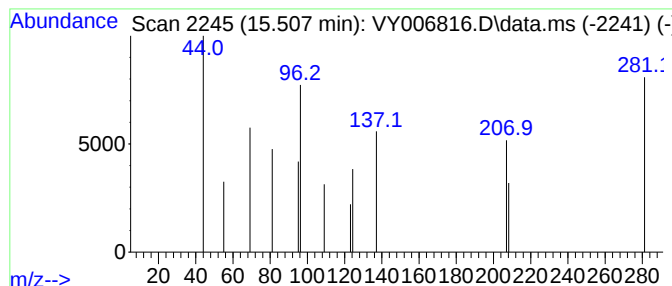
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown15.507 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.507	15.91 ug/l	1291	1,4-Dichlorobenzene-d4	13.434

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(Cyclododec-1-en-1-yl)ethanone	208	C14H24O	065938-08-1	10		
2	(Dimethylsulfamoyl)amine	124	C2H8N2O2S	003984-14-3	9		
3	2-Cyclohexen-1-one, 3,4-dimethyl-	124	C8H12O	1000197-00-4	9		
4	3-(1-Methylhept-1-enyl)-5-methyl...	208	C13H20O2	1000284-50-5	9		
5	Cyclopropane carboxamide, 2-cycl...	207	C13H21NO	331416-19-4	9		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown13.861	13.861	11.4	ug/l	926	4	13.434	4057	50.0
unknown15.507	15.507	15.9	ug/l	1291	4	13.434	4057	50.0