

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM051021\
 Data File : BM029956.D
 Acq On : 11 May 2021 23:14
 Operator : CG/JU
 Sample : M2197-12
 Misc :
 ALS Vial : 55 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 YARH8

Integration Parameters: LSCINT.P

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

Filtering: 5
 Min Area: 0.1 % 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:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM050721.M
 Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.016	18	22	27	rBV	135974	186682	4.66%	0.491%
2	3.057	27	29	38	rVB	42226	60290	1.50%	0.158%
3	3.687	131	136	144	rVB	22905	39371	0.98%	0.103%
4	3.775	148	151	155	rVB3	8722	10886	0.27%	0.029%
5	3.881	166	169	173	rVB4	9067	11482	0.29%	0.030%
6	4.210	221	225	229	rVB6	3992	6284	0.16%	0.017%
7	4.293	234	239	245	rVV	59799	86484	2.16%	0.227%
8	5.951	516	521	526	rBV4	6531	12239	0.31%	0.032%
9	6.692	642	647	650	rBV	23834	33423	0.83%	0.088%
10	6.739	650	655	669	rVB	115934	257326	6.42%	0.676%
11	6.892	675	681	701	rBV	447993	809963	20.22%	2.129%
12	7.081	707	713	726	rBV	556774	954598	23.83%	2.509%
13	7.545	785	792	801	rBV	472182	779981	19.47%	2.050%
14	8.263	908	914	933	rBV	373300	731383	18.26%	1.922%
15	8.698	980	988	1012	rBV	592235	1115839	27.85%	2.933%
16	9.116	1054	1059	1065	rVB	53248	79021	1.97%	0.208%
17	9.416	1103	1110	1132	rBV	507473	932970	23.29%	2.452%
18	9.951	1195	1201	1226	rBV	577512	1316763	32.87%	3.461%
19	10.275	1250	1256	1257	rBV2	16296	20484	0.51%	0.054%
20	10.316	1257	1263	1274	rVB	680516	1182468	29.52%	3.108%
21	10.492	1286	1293	1305	rBV3	32925	97941	2.44%	0.257%
22	11.604	1476	1482	1487	rBV2	13977	23033	0.57%	0.061%
23	11.939	1533	1539	1545	rBV4	6752	14845	0.37%	0.039%
24	12.539	1636	1641	1646	rBV6	4887	8205	0.20%	0.022%
25	12.727	1670	1673	1681	rVB5	2731	5425	0.14%	0.014%
26	12.798	1681	1685	1691	rBV4	6027	10012	0.25%	0.026%
27	13.021	1718	1723	1728	rBV	13965	20738	0.52%	0.055%
28	13.098	1731	1736	1743	rVB4	4580	8490	0.21%	0.022%
29	13.616	1817	1824	1829	rBV	1596133	2278173	56.87%	5.988%
30	13.663	1829	1832	1841	rVB	66683	107394	2.68%	0.282%
31	13.886	1862	1870	1886	rBV	1836490	2777367	69.33%	7.300%
32	14.110	1901	1908	1913	rVB5	8124	14271	0.36%	0.038%
33	14.192	1916	1922	1940	rVB	1100222	1621937	40.49%	4.263%
34	14.463	1959	1968	1969	rBV5	16780	24747	0.62%	0.065%

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35	14.833	2028	2031	2037	rBV8	2168	4098	0.10%	0.011%
36	15.033	2056	2065	2075	rBV	61377	102112	2.55%	0.268%
37	15.192	2085	2092	2109	rBV	2446426	3460682	86.38%	9.096%
38	15.327	2109	2115	2129	rVV	640835	988582	24.68%	2.598%
39	15.433	2129	2133	2137	rVB2	26261	41587	1.04%	0.109%
40	15.574	2153	2157	2159	rVV5	3843	4777	0.12%	0.013%
41	15.621	2162	2165	2169	rVB5	2954	4647	0.12%	0.012%
42	15.874	2203	2208	2211	rBV7	3602	5844	0.15%	0.015%
43	15.921	2214	2216	2221	rVV5	3564	5202	0.13%	0.014%
44	15.974	2222	2225	2231	rVB5	8795	14521	0.36%	0.038%
45	16.180	2256	2260	2265	rVB	15562	19477	0.49%	0.051%
46	16.274	2270	2276	2280	rBV6	3122	5123	0.13%	0.013%
47	16.333	2280	2286	2291	rVB5	4124	8078	0.20%	0.021%
48	16.621	2332	2335	2339	rVB6	4828	5958	0.15%	0.016%
49	16.733	2348	2354	2357	rBV6	4351	7887	0.20%	0.021%
50	16.939	2383	2389	2399	rBV	1220023	1743546	43.52%	4.583%
51	17.039	2399	2406	2421	rVV	2521200	3660106	91.36%	9.621%
52	17.239	2437	2440	2444	rVB3	4040	5727	0.14%	0.015%
53	17.615	2502	2504	2510	rVB7	3131	4350	0.11%	0.011%
54	17.845	2539	2543	2553	rBV	113228	204751	5.11%	0.538%
55	17.921	2553	2556	2561	rVB2	15767	22961	0.57%	0.060%
56	18.533	2657	2660	2663	rBV5	3360	4554	0.11%	0.012%
57	18.974	2731	2735	2740	rBV2	22600	32958	0.82%	0.087%
58	19.139	2758	2763	2771	rBV2	52159	92616	2.31%	0.243%
59	19.227	2774	2778	2781	rVV	19896	27146	0.68%	0.071%
60	19.274	2781	2786	2791	rVV	280304	325526	8.13%	0.856%
61	19.339	2791	2797	2811	rVB	2976443	4006226	100.00%	10.530%
62	20.850	3050	3054	3063	rBV	240021	389469	9.72%	1.024%
63	21.127	3096	3101	3112	rBV	1167330	1644968	41.06%	4.324%
64	21.956	3239	3242	3247	rVB	193454	229223	5.72%	0.603%
65	23.144	3437	3444	3456	rBV	2047331	3724278	92.96%	9.789%
66	23.280	3461	3467	3478	rVB2	862236	1606915	40.11%	4.224%

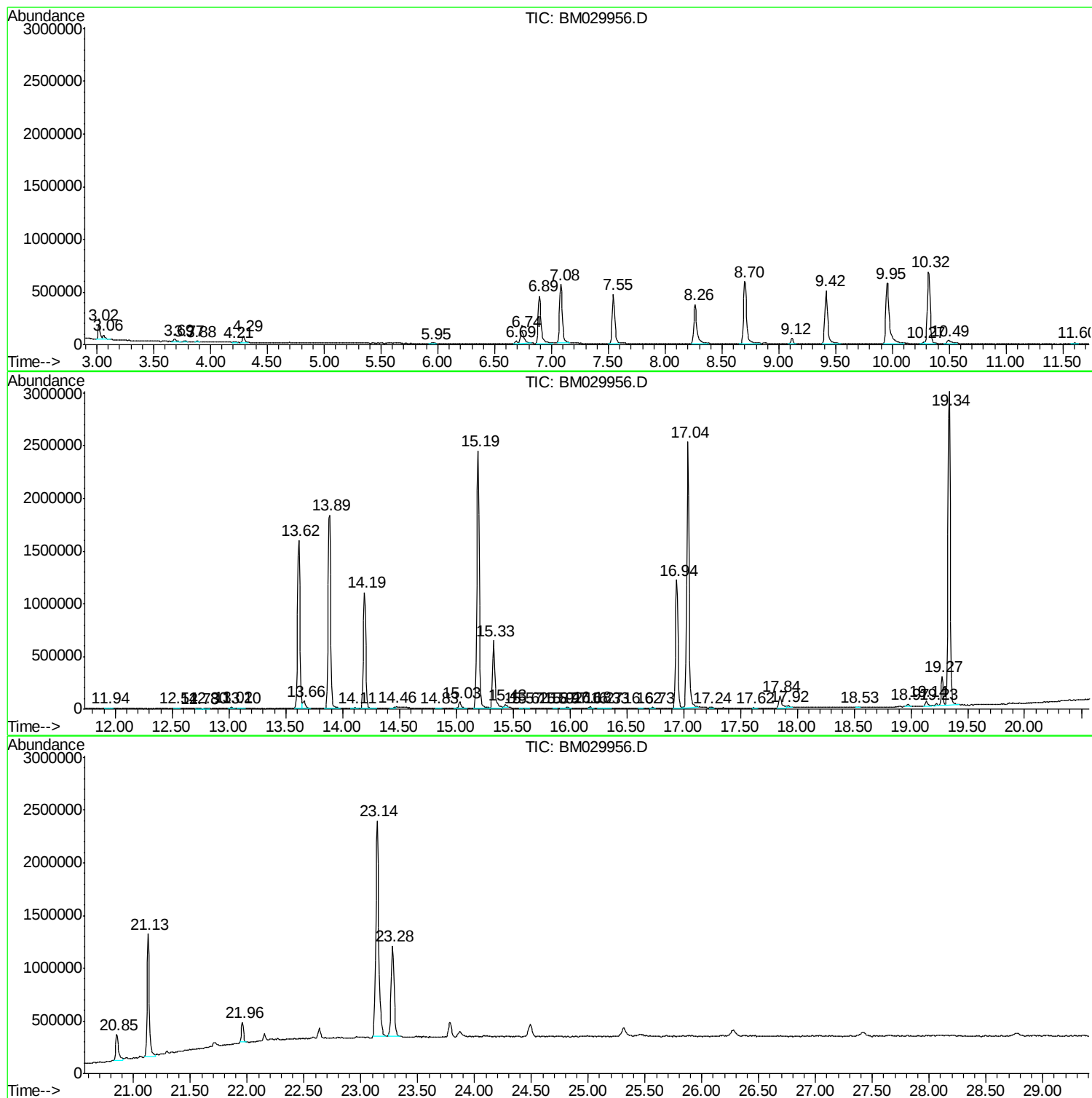
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Quant Title : SVOA CALIBRATION

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



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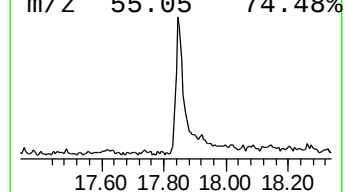
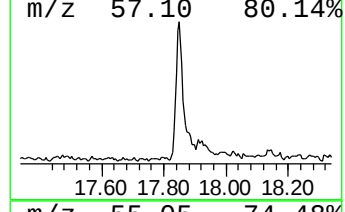
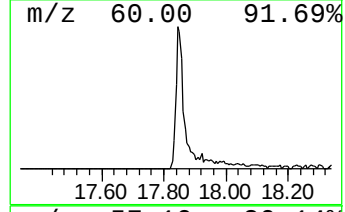
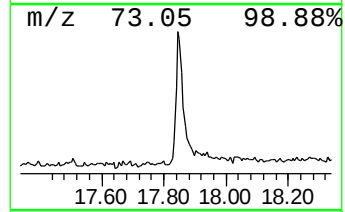
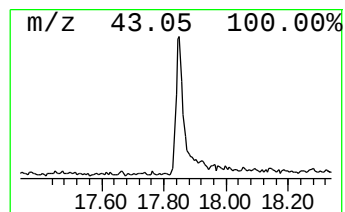
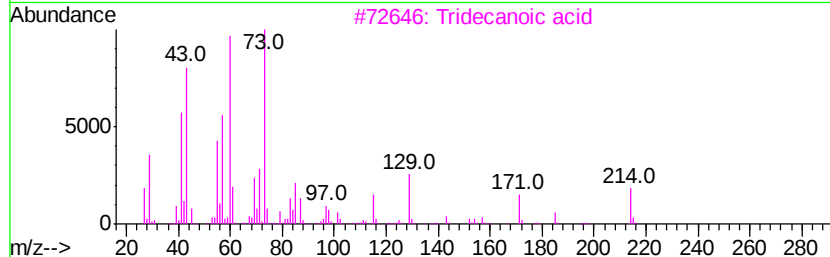
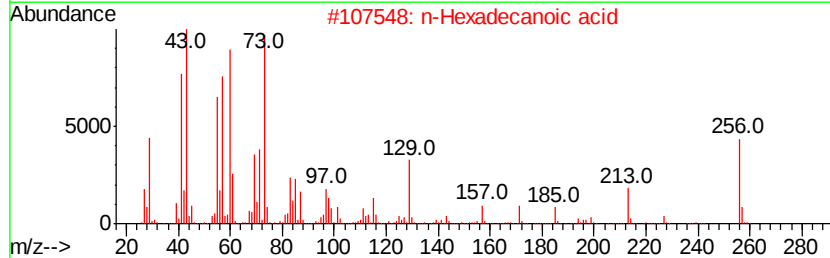
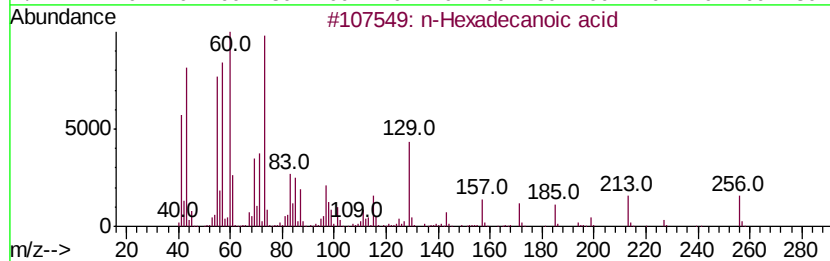
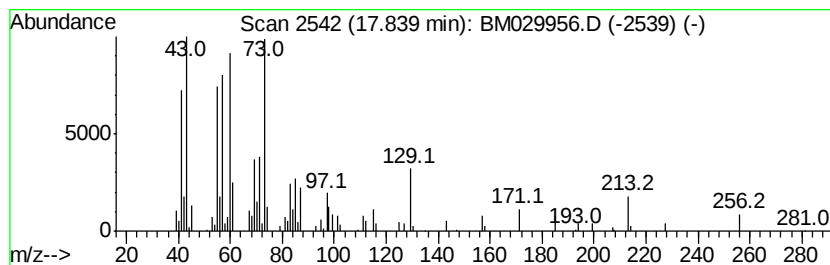
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Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.84	2.35 ng/ul	204751	Phenanthrene-d10	16.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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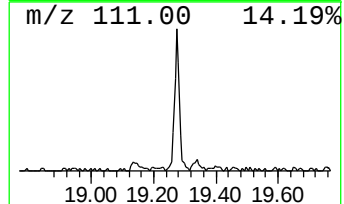
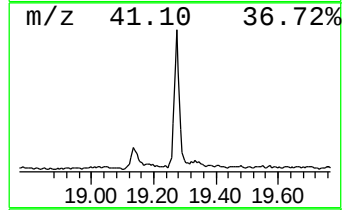
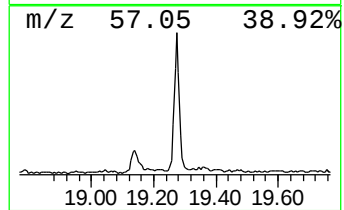
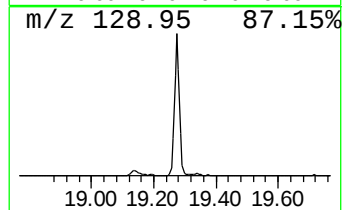
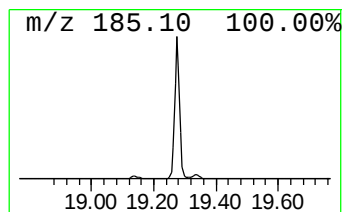
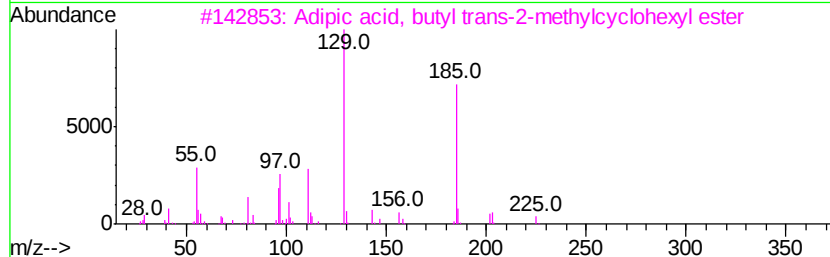
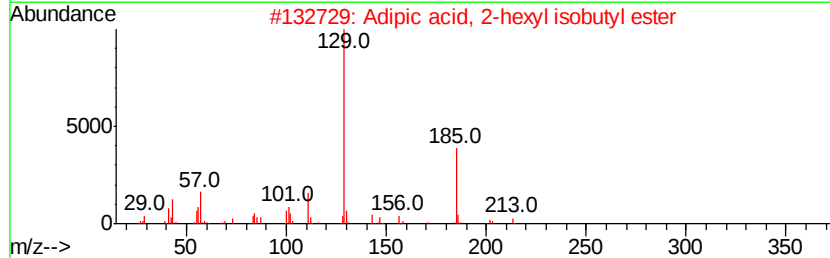
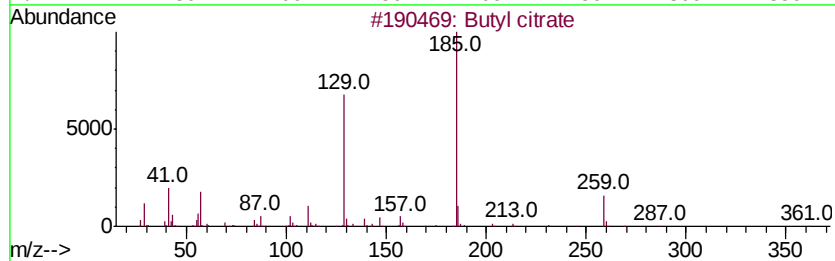
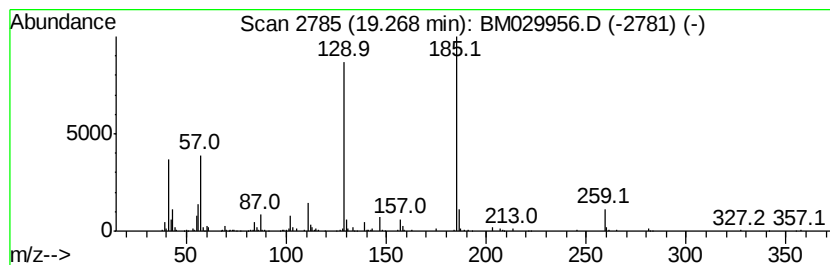
Instrument :
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	3.96 ng/ul	325526	Chrysene-d12	21.13
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	81
2	Adipic acid, 2-hexyl isobutyl ester	286 C16H30O4	1000353-70-9	78
3	Adipic acid, butyl trans-2-methy...	298 C17H30O4	1000324-74-6	72
4	Adipic acid, butyl 2-decyl ester	342 C20H38O4	1000353-59-7	72
5	Adipic acid, butyl 4-heptyl ester	300 C17H32O4	1000349-73-7	64



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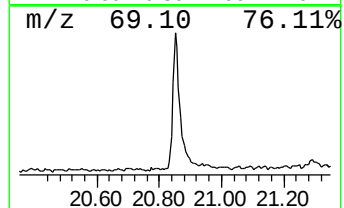
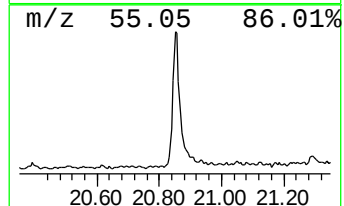
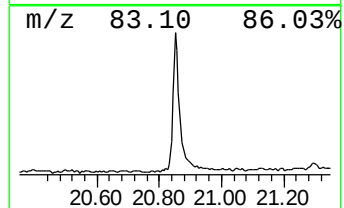
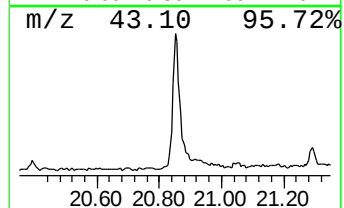
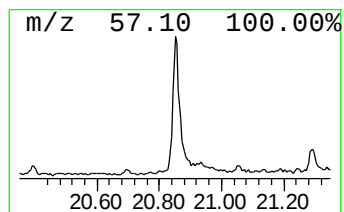
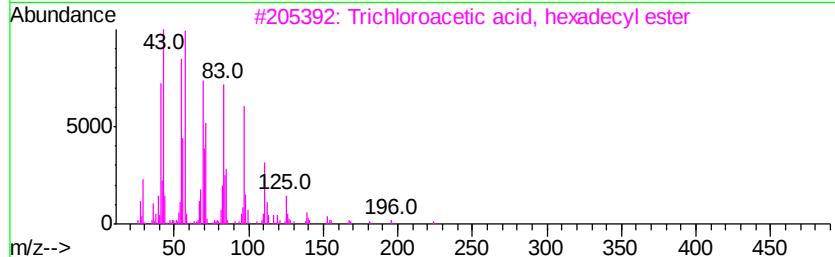
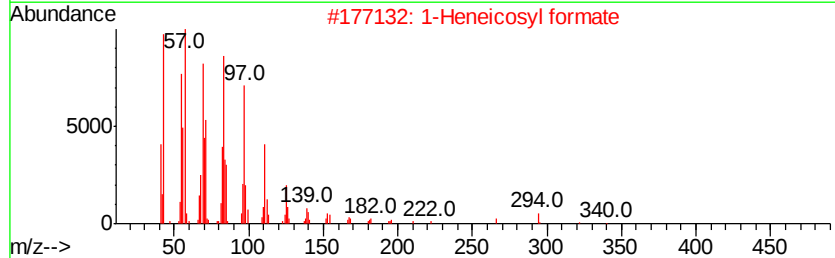
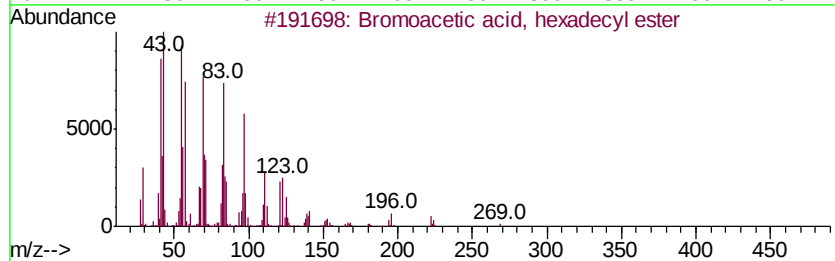
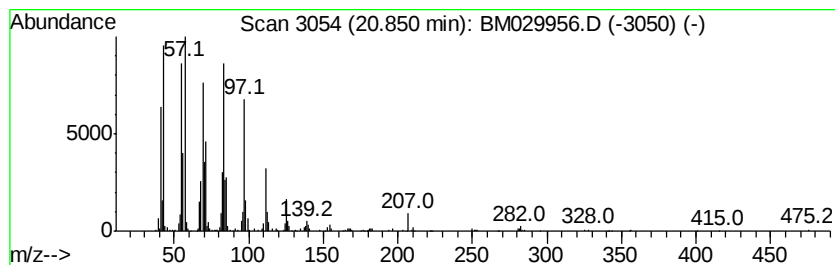
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	4.74 ng/ul	389469	Chrysene-d12	21.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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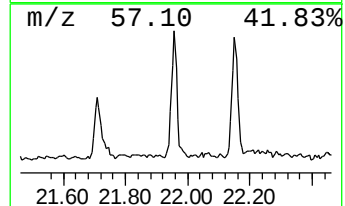
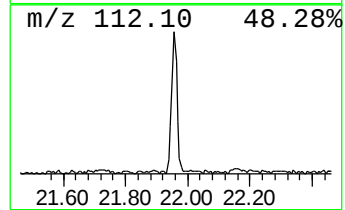
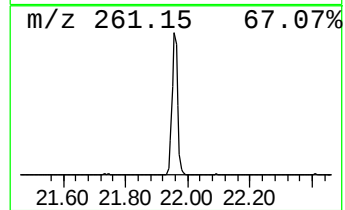
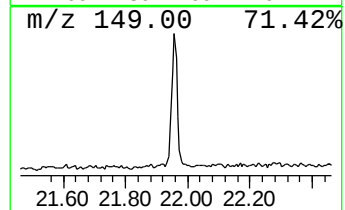
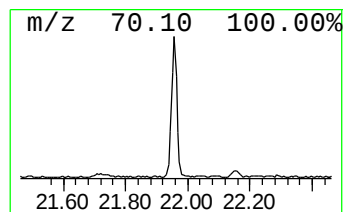
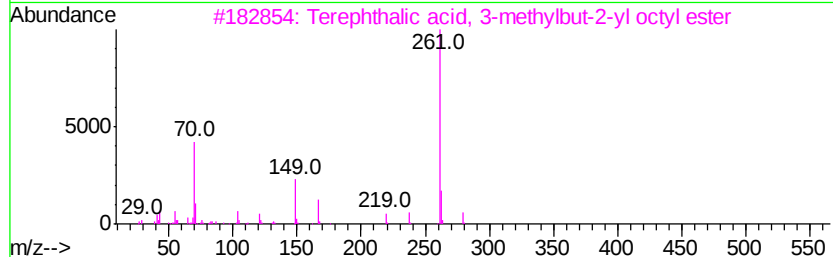
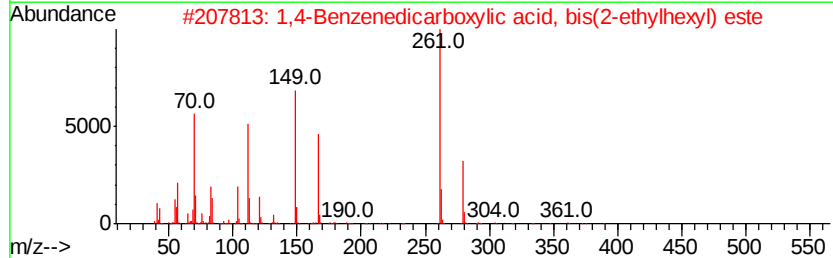
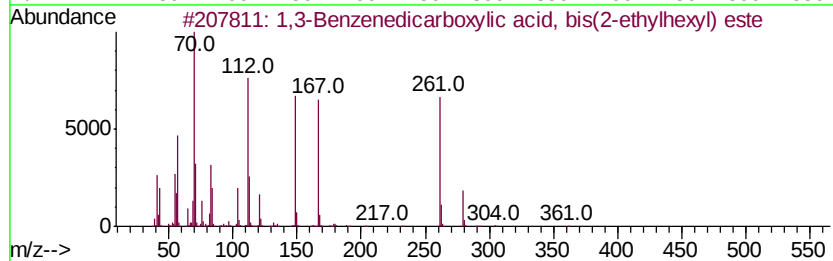
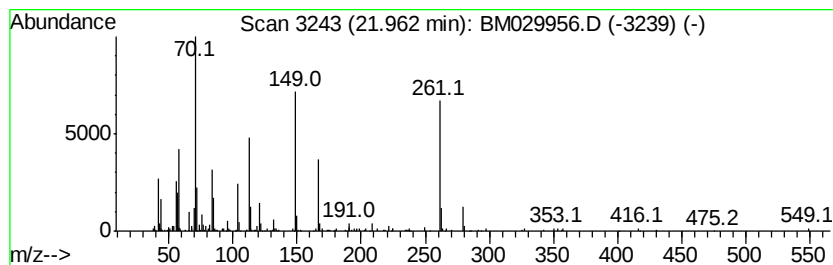
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1,3-Benzenedicarboxylic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.96	2.79 ng/ul	229223	Chrysene-d12	21.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	72
3			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	47
4			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	46
5			2-(Decyloxycarbonyl)benzoic acid	306	C18H26O4	1000373-53-2	38



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM050721.M
Quant Title : SVOA CALIBRATION

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-Hexadecanoic acid	17.84	2.4	ng/ul	204751	4	16.94	1743550	20.0
Butyl citrate	19.27	4.0	ng/ul	325526	5	21.13	1644970	20.0
Bromoacetic acid,...	20.85	4.7	ng/ul	389469	5	21.13	1644970	20.0
1,3-Benzenedicarb...	21.96	2.8	ng/ul	229223	5	21.13	1644970	20.0