

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
 Data File : BP017479.D
 Acq On : 02 Oct 2023 16:16
 Operator : MA/JU
 Sample : 04562-07 50X
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCJL6

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP017479.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.040	158	162	166	rVB	19779	26811	1.87%	0.274%
2	5.346	380	384	390	rBV3	8601	14216	0.99%	0.145%
3	5.746	449	452	454	rBV4	2962	4461	0.31%	0.046%
4	5.969	484	490	493	rBV8	3014	5032	0.35%	0.051%
5	6.593	592	596	601	rBV8	2922	4782	0.33%	0.049%
6	6.928	646	653	661	rBV	37195	67599	4.72%	0.690%
7	7.116	680	685	691	rVB9	3577	7347	0.51%	0.075%
8	7.293	711	715	722	rVV3	9690	16462	1.15%	0.168%
9	7.381	727	730	736	rVB6	5655	7804	0.54%	0.080%
10	7.469	740	745	752	rVB3	9850	17077	1.19%	0.174%
11	7.622	767	771	775	rVB6	2131	3510	0.24%	0.036%
12	7.946	819	826	836	rBV	387671	603775	42.13%	6.161%
13	8.522	915	924	933	rBV	71080	138325	9.65%	1.411%
14	8.675	945	950	953	rBV4	8610	14045	0.98%	0.143%
15	9.022	1007	1009	1014	rVB5	3076	3700	0.26%	0.038%
16	9.157	1027	1032	1037	rBV3	10762	18332	1.28%	0.187%
17	9.263	1046	1050	1051	rBV3	2146	2415	0.17%	0.025%
18	9.346	1062	1064	1068	rVB5	2512	2340	0.16%	0.024%
19	9.522	1089	1094	1098	rBV7	2490	3482	0.24%	0.036%
20	9.852	1147	1150	1151	rBV3	2063	2336	0.16%	0.024%
21	9.881	1151	1155	1160	rVB7	7190	11858	0.83%	0.121%
22	10.081	1179	1189	1195	rBV2	105731	196299	13.70%	2.003%
23	10.281	1219	1223	1225	rBV6	1952	3230	0.23%	0.033%
24	10.416	1240	1246	1251	rBV3	9983	21912	1.53%	0.224%
25	10.534	1263	1266	1267	rVV3	3091	3220	0.22%	0.033%
26	10.557	1267	1270	1274	rVV6	3675	6104	0.43%	0.062%
27	10.610	1274	1279	1284	rVB6	4889	8631	0.60%	0.088%
28	10.787	1300	1309	1324	rBV	507122	846614	59.08%	8.639%
29	11.493	1423	1429	1430	rBV6	2842	3694	0.26%	0.038%
30	11.563	1430	1441	1452	rVV	78978	149613	10.44%	1.527%
31	11.922	1501	1502	1505	rBV3	2556	2362	0.16%	0.024%
32	12.028	1515	1520	1522	rVV6	2408	4402	0.31%	0.045%
33	12.057	1522	1525	1528	rVV4	2557	3028	0.21%	0.031%
34	12.093	1528	1531	1536	rVV6	4402	6339	0.44%	0.065%
35	12.698	1631	1634	1638	rVB6	1488	2419	0.17%	0.025%
36	12.893	1661	1667	1668	rBV6	3674	4692	0.33%	0.048%

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37	13.116	1696	1705	1712	rVB7	13375	37530	2.62%	0.383%
38	13.304	1731	1737	1746	rVV4	22853	66252	4.62%	0.676%
39	13.363	1746	1747	1754	rVV4	10661	15939	1.11%	0.163%
40	13.428	1754	1758	1761	rVV3	9624	15983	1.12%	0.163%

41	13.463	1761	1764	1771	rVB5	8479	15889	1.11%	0.162%
42	13.569	1777	1782	1791	rBV5	16497	25901	1.81%	0.264%
43	13.763	1812	1815	1819	rVB5	1870	2541	0.18%	0.026%
44	13.863	1828	1832	1833	rVV4	3127	3305	0.23%	0.034%
45	14.057	1857	1865	1870	rBV2	24375	39522	2.76%	0.403%

46	14.110	1872	1874	1880	rVB6	3311	5027	0.35%	0.051%
47	14.245	1887	1897	1905	rBV4	46544	88596	6.18%	0.904%
48	14.340	1908	1913	1918	rBV	27351	38407	2.68%	0.392%
49	14.410	1920	1925	1932	rBV4	18044	46291	3.23%	0.472%
50	14.463	1932	1934	1939	rVB4	7105	9290	0.65%	0.095%

51	14.522	1939	1944	1948	rBV2	293763	540528	37.72%	5.515%
52	14.640	1959	1964	1972	rVB	774211	1103017	76.97%	11.255%
53	14.722	1976	1978	1982	rVB5	6457	7116	0.50%	0.073%
54	14.792	1987	1990	1993	rVB5	3112	3762	0.26%	0.038%
55	14.845	1995	1999	2003	rBV7	3622	6677	0.47%	0.068%

56	14.951	2014	2017	2019	rBV4	2146	2404	0.17%	0.025%
57	15.034	2027	2031	2036	rBV7	6821	13767	0.96%	0.140%
58	15.098	2036	2042	2046	rVB8	4064	7869	0.55%	0.080%
59	15.134	2046	2048	2052	rVB5	2975	3872	0.27%	0.040%
60	15.187	2052	2057	2058	rBV5	3163	4946	0.35%	0.050%

61	15.210	2059	2061	2066	rVB6	3572	4332	0.30%	0.044%
62	15.328	2077	2081	2085	rVB4	8700	11136	0.78%	0.114%
63	15.392	2087	2092	2096	rBV7	7053	13301	0.93%	0.136%
64	15.487	2104	2108	2117	rVB9	5933	13165	0.92%	0.134%
65	15.545	2117	2118	2122	rVB5	3949	3500	0.24%	0.036%

66	15.598	2122	2127	2129	rBV6	3113	5683	0.40%	0.058%
67	15.645	2129	2135	2146	rVB	37495	69811	4.87%	0.712%
68	15.745	2150	2152	2153	rBV2	2993	2546	0.18%	0.026%
69	15.787	2153	2159	2165	rVB7	9212	17907	1.25%	0.183%
70	15.875	2172	2174	2175	rBV2	3219	2573	0.18%	0.026%

71	15.898	2175	2178	2180	rVB3	2680	3339	0.23%	0.034%
72	15.987	2191	2193	2196	rBV4	2533	3098	0.22%	0.032%
73	16.022	2196	2199	2201	rVV4	3441	4519	0.32%	0.046%
74	16.081	2205	2209	2210	rBV4	2997	4005	0.28%	0.041%
75	16.104	2210	2213	2219	rVV6	9120	15141	1.06%	0.154%

76	16.169	2219	2224	2233	rVB10	17319	26727	1.87%	0.273%
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77	16.292	2242	2245	2248	rBV5	3148	5548	0.39%	0.057%
78	16.357	2249	2256	2257	rVV	73011	87654	6.12%	0.894%
79	16.375	2257	2259	2268	rVV	83182	141213	9.85%	1.441%
80	16.439	2268	2270	2277	rVV	13129	23856	1.66%	0.243%
81	16.592	2293	2296	2299	rBV3	5113	6336	0.44%	0.065%
82	16.634	2299	2303	2310	rVB4	8971	15214	1.06%	0.155%
83	16.745	2314	2322	2326	rBV5	5221	13833	0.97%	0.141%
84	16.951	2354	2357	2362	rVB	7059	8398	0.59%	0.086%
85	17.075	2374	2378	2381	rBV6	3707	6492	0.45%	0.066%
86	17.210	2399	2401	2406	rVV5	2371	3591	0.25%	0.037%
87	17.269	2408	2411	2417	rVB2	9379	14763	1.03%	0.151%
88	17.351	2423	2425	2428	rBV4	2122	3249	0.23%	0.033%
89	17.428	2431	2438	2449	rVV	962242	1322170	92.27%	13.491%
90	17.528	2450	2455	2463	rVB2	36687	59554	4.16%	0.608%
91	17.639	2472	2474	2477	rBV4	2540	2749	0.19%	0.028%
92	18.022	2536	2539	2540	rBV3	2936	2760	0.19%	0.028%
93	18.286	2580	2584	2585	rBV4	4883	6700	0.47%	0.068%
94	19.416	2773	2776	2781	rBV	68667	78397	5.47%	0.800%
95	19.657	2812	2817	2820	rBV	242258	273597	19.09%	2.792%
96	19.775	2833	2837	2843	rBV2	58540	88551	6.18%	0.904%
97	20.475	2953	2956	2960	rBV3	40415	47990	3.35%	0.490%
98	20.680	2988	2991	2996	rBV	187501	212456	14.83%	2.168%
99	21.557	3135	3140	3146	rBV	1065977	1398646	97.60%	14.272%
100	24.127	3571	3577	3589	rVB	681930	1432966	100.00%	14.622%

Sum of corrected areas: 9800165

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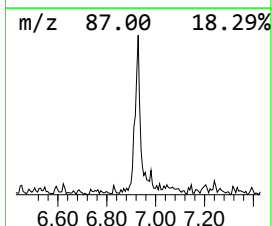
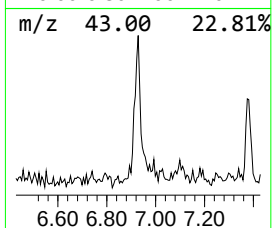
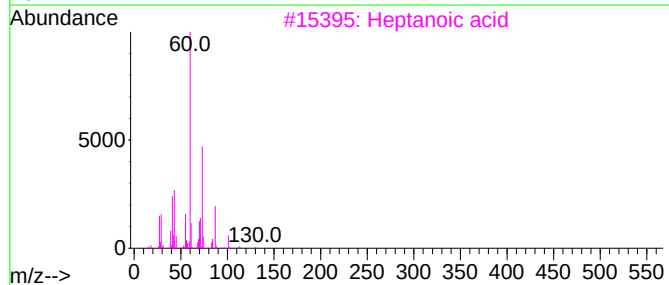
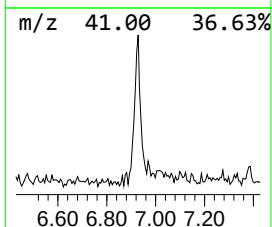
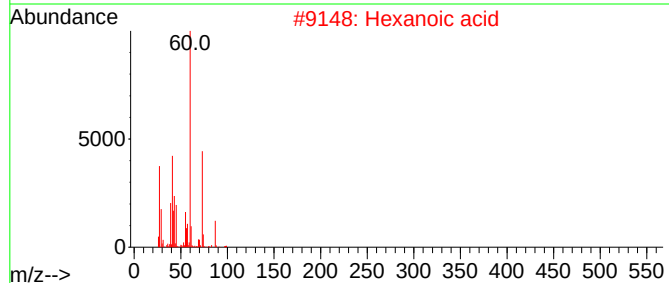
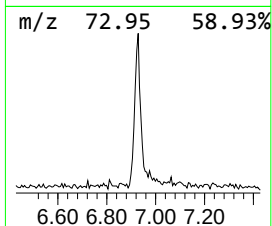
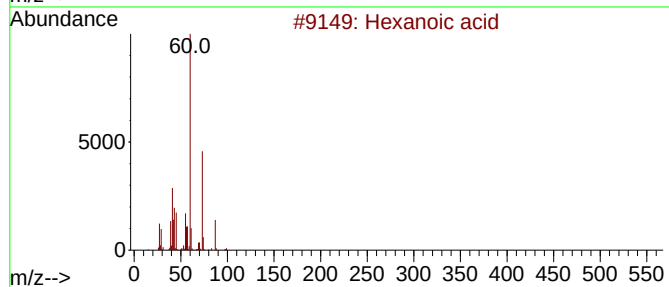
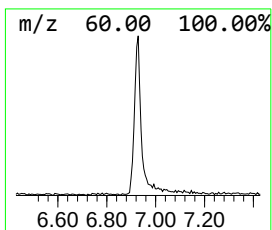
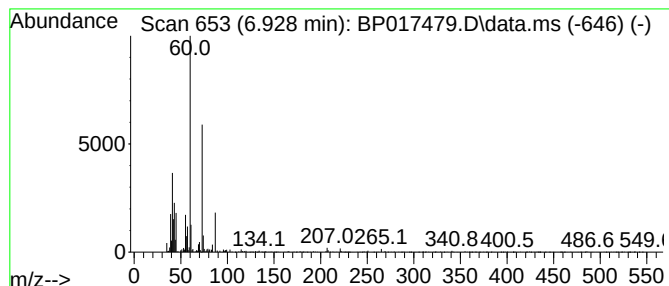
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Hexanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	2.24 ng/ul	67599	1,4-Dichlorobenzene-d4	7.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid	116	C6H12O2	000142-62-1	86
2			Hexanoic acid	116	C6H12O2	000142-62-1	83
3			Heptanoic acid	130	C7H14O2	000111-14-8	80
4			Heptanoic acid	130	C7H14O2	000111-14-8	78
5			Hexanoic acid	116	C6H12O2	000142-62-1	78



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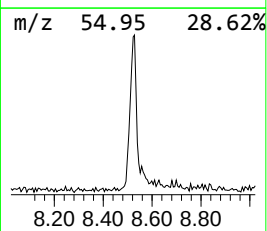
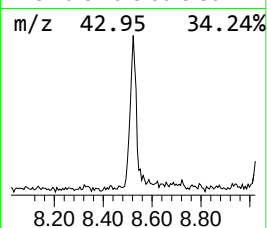
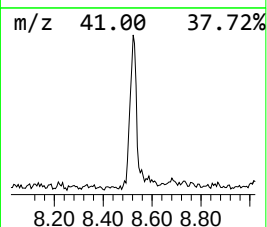
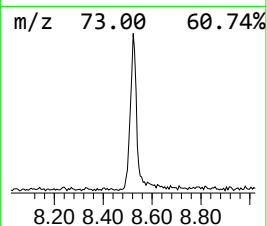
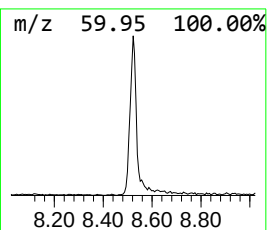
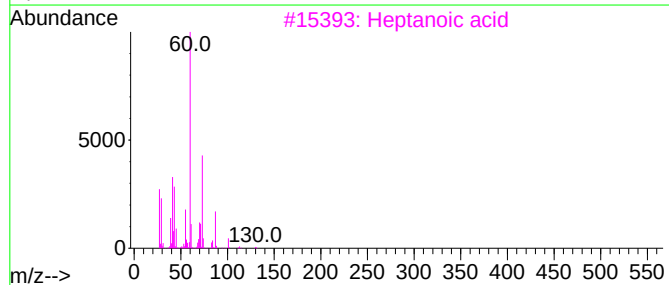
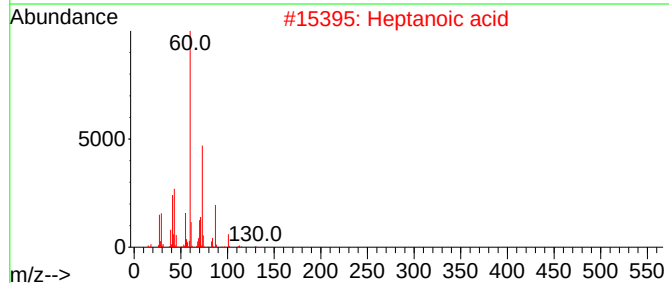
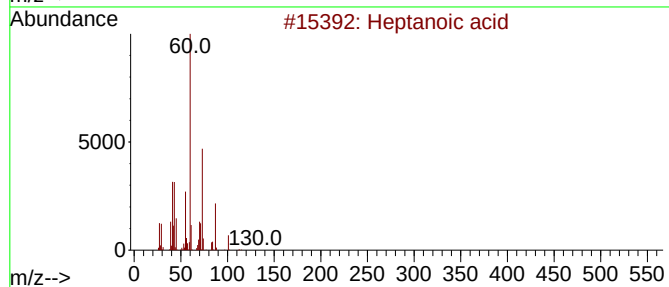
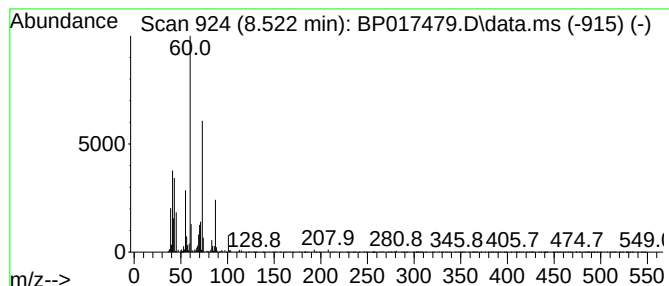
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Heptanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.522	4.58 ng/ul	138325	1,4-Dichlorobenzene-d4	7.946

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	90
2			Heptanoic acid	130	C7H14O2	000111-14-8	90
3			Heptanoic acid	130	C7H14O2	000111-14-8	83
4			Heptanoic acid	130	C7H14O2	000111-14-8	64
5			Hexanoic acid	116	C6H12O2	000142-62-1	64



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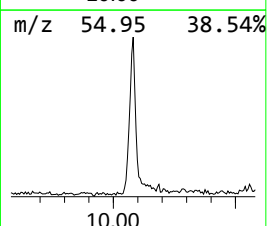
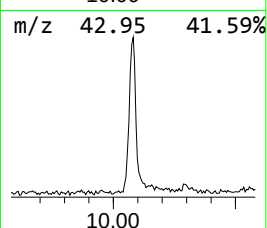
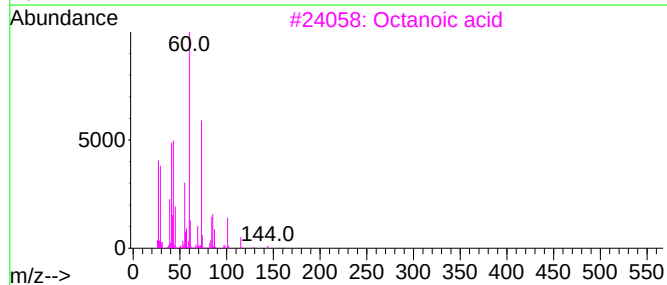
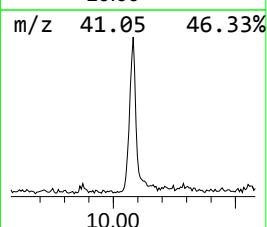
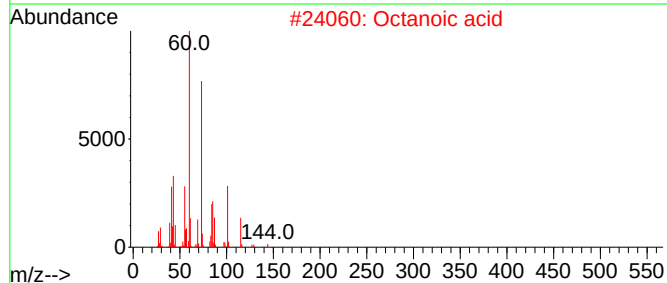
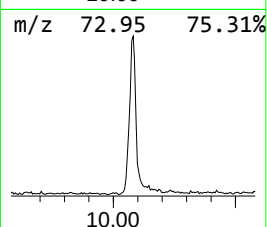
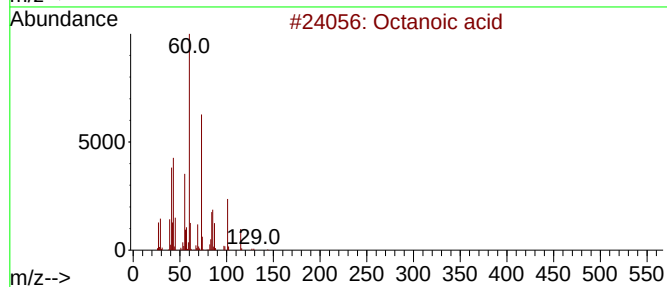
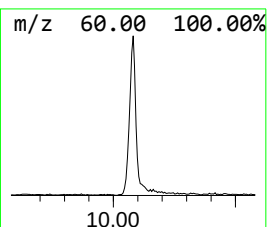
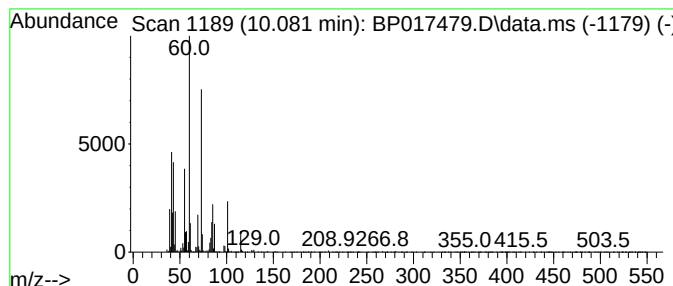
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.081	4.64 ng/ul	196299	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	94
2			Octanoic acid	144	C8H16O2	000124-07-2	90
3			Octanoic acid	144	C8H16O2	000124-07-2	86
4			Octanoic acid	144	C8H16O2	000124-07-2	72
5			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	64



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DCJL6

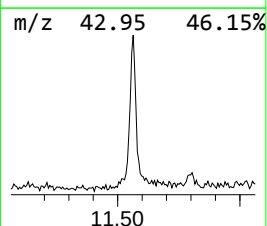
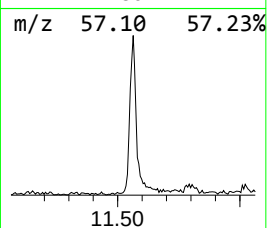
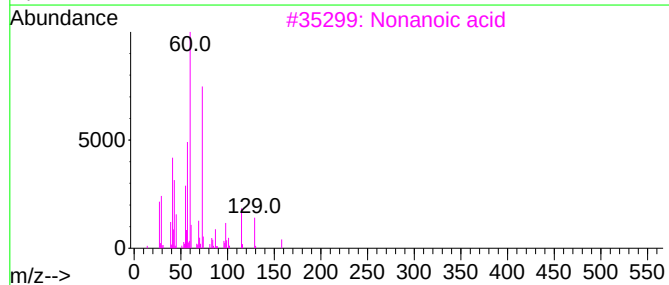
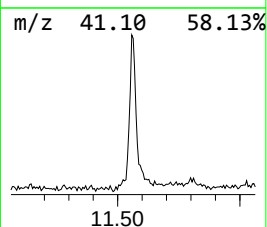
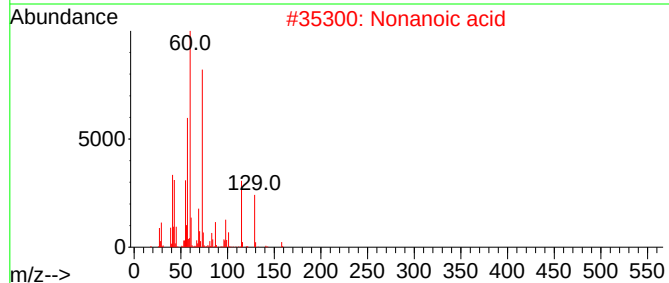
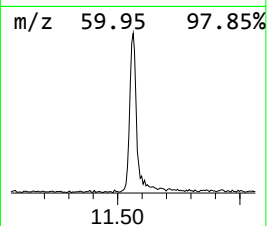
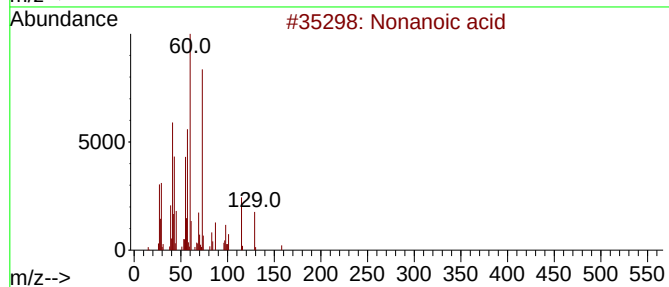
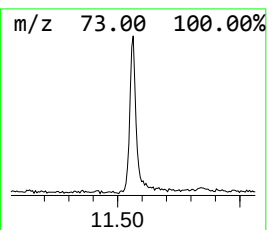
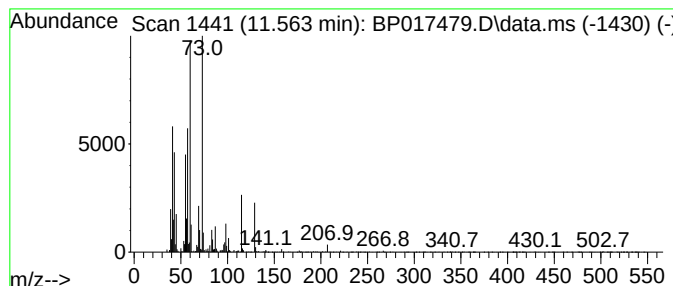
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Nonanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.563	3.53 ng/ul	149613	Naphthalene-d8	10.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	91
2			Nonanoic acid	158	C9H18O2	000112-05-0	72
3			Nonanoic acid	158	C9H18O2	000112-05-0	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
Data File : BP017479.D
Acq On : 02 Oct 2023 16:16
Operator : MA/JU
Sample : 04562-07 50X
Misc :
ALS Vial : 4 Sample Multiplier: 1

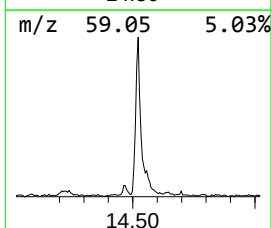
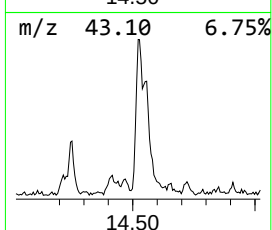
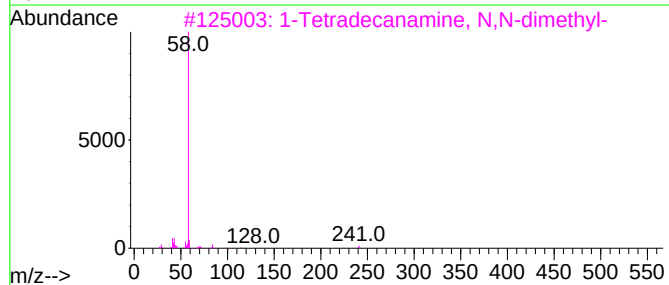
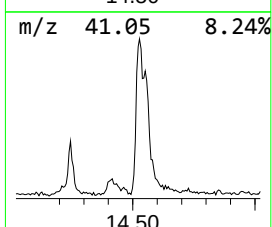
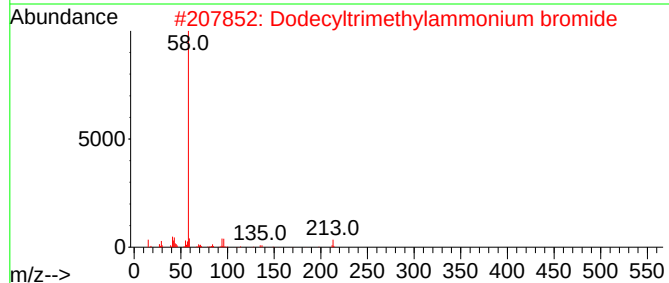
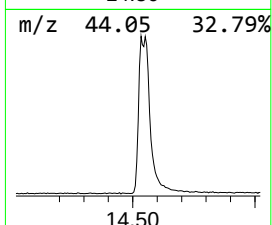
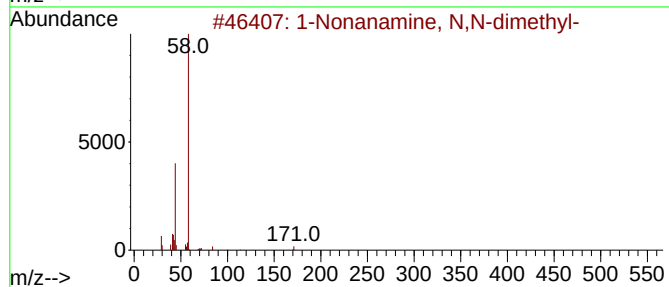
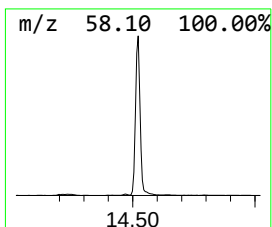
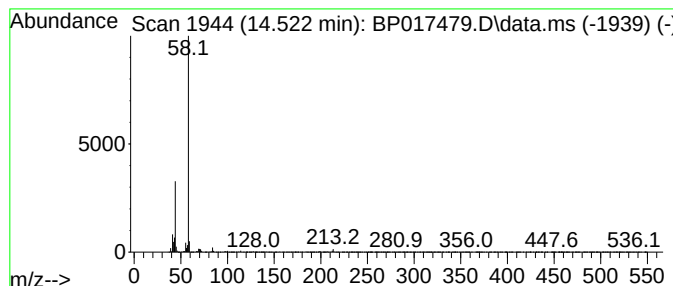
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Nonanamine, N,N-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.522	9.80 ng/ul	540528	Acenaphthene-d10	14.640	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanamine, N,N-dimethyl-	171	C11H25N	017373-27-2	64
2	Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	59
3	1-Tetradecanamine, N,N-dimethyl-	241	C16H35N	000112-75-4	59
4	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	59
5	10-Aminodecanoic acid, N,N,O-tri...	229	C13H27NO2	874761-97-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
Data File : BP017479.D
Acq On : 02 Oct 2023 16:16
Operator : MA/JU
Sample : 04562-07 50X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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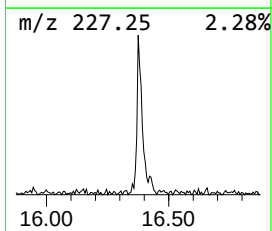
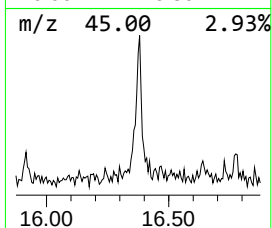
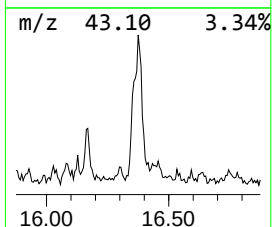
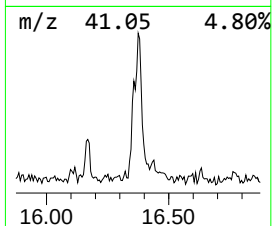
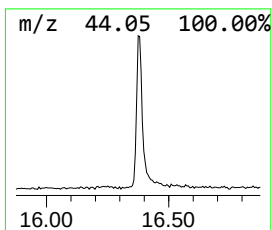
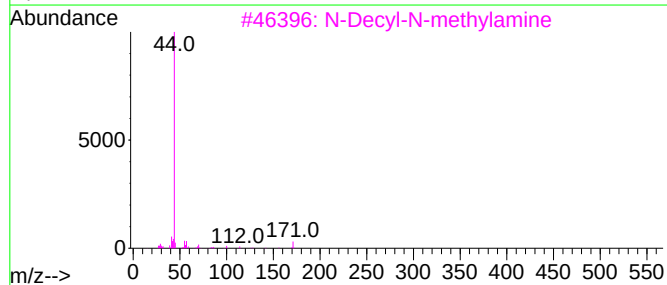
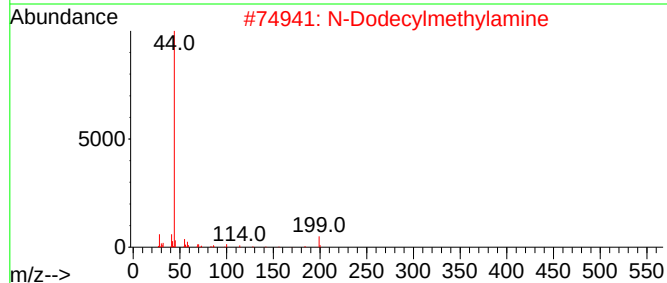
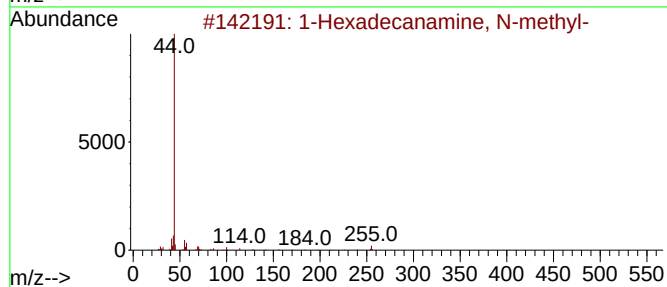
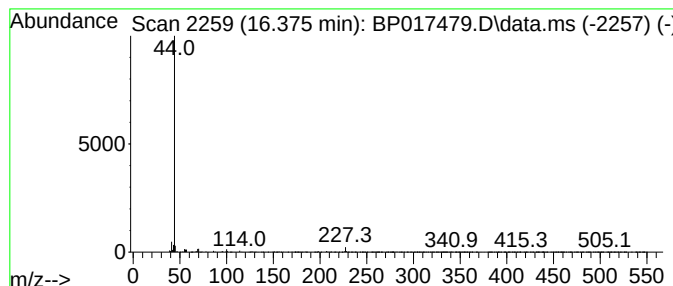
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Hexadecanamine, N-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.375	2.14 ng/ul	141213	Phenanthrene-d10	17.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanamine, N-methyl-	255	C17H37N	013417-08-8	56
2			N-Dodecylmethylamine	199	C13H29N	1000342-26-1	50
3			N-Decyl-N-methylamine	171	C11H25N	007516-82-7	40
4			12-Methylaminolauric acid	229	C13H27NO2	007408-81-3	39
5			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	17



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
Data File : BP017479.D
Acq On : 02 Oct 2023 16:16
Operator : MA/JU
Sample : 04562-07 50X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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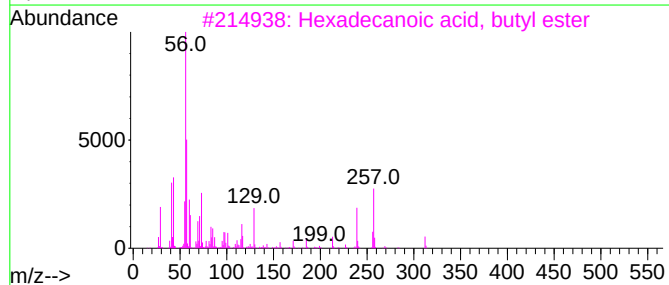
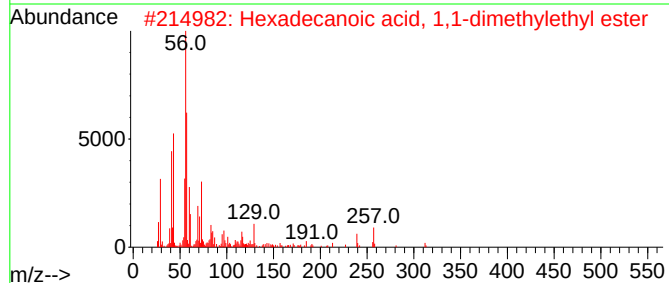
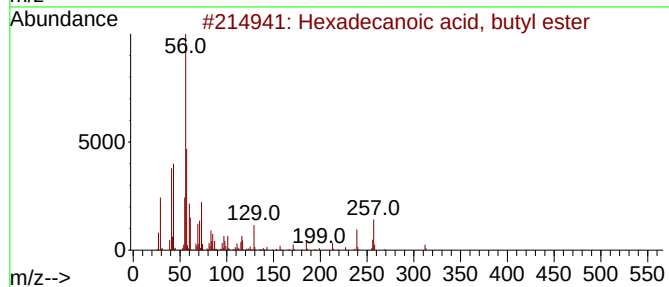
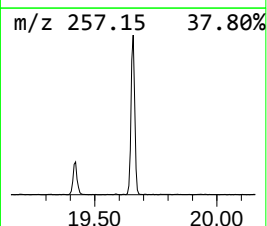
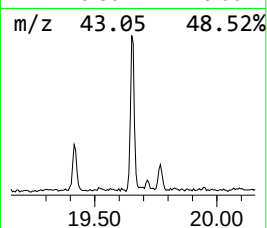
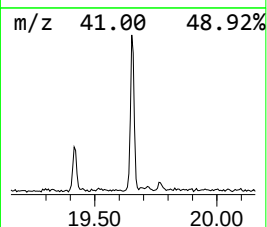
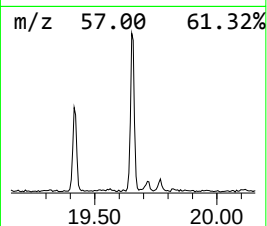
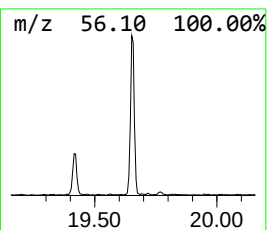
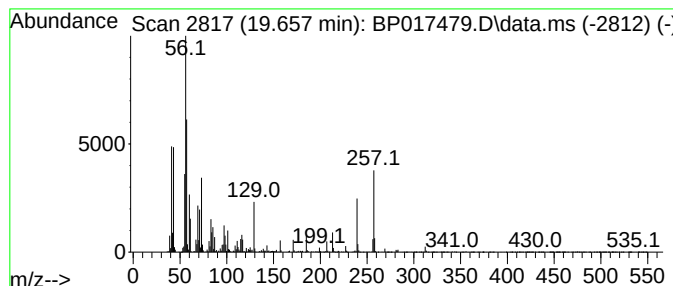
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.657	3.91 ng/ul	273597	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
3			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
4			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	86
5			Nipecotic acid	129	C6H11NO2	000498-95-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
Data File : BP017479.D
Acq On : 02 Oct 2023 16:16
Operator : MA/JU
Sample : 04562-07 50X
Misc :
ALS Vial : 4 Sample Multiplier: 1

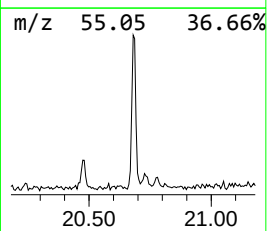
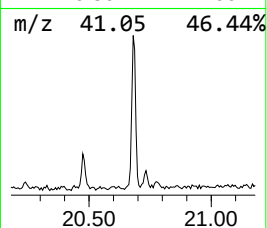
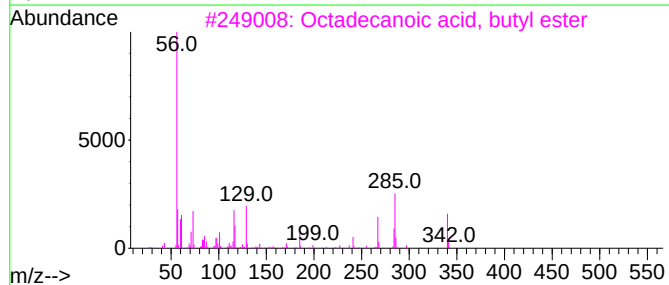
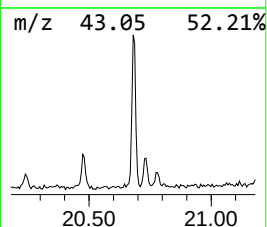
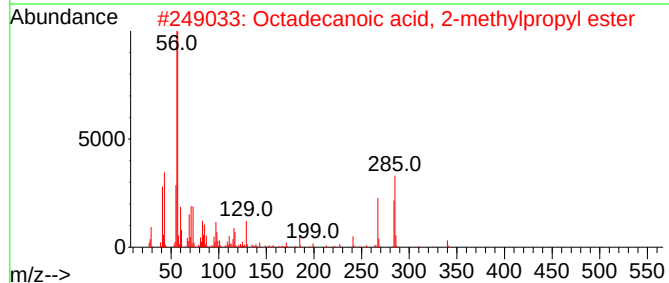
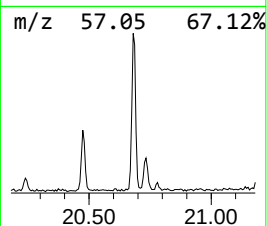
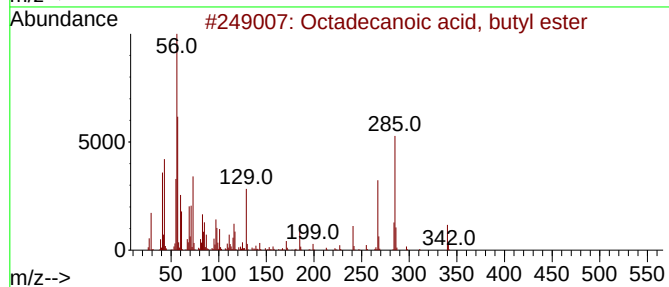
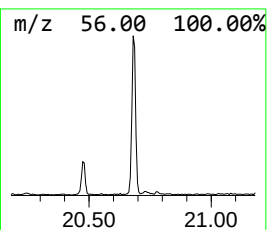
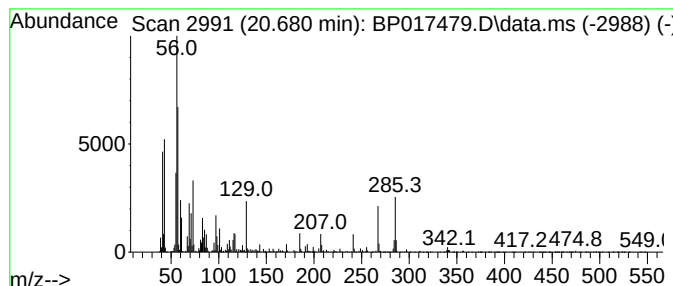
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.680	3.04 ng/ul	212456	Chrysene-d12	21.557	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	99
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	93
3	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	80
4	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	74
5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100223\
Data File : BP017479.D
Acq On : 02 Oct 2023 16:16
Operator : MA/JU
Sample : 04562-07 50X
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCJL6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092023.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanoic acid	6.928	2.2	ng/ul	67599	1	7.946	603775	20.0
Heptanoic acid	8.522	4.6	ng/ul	138325	1	7.946	603775	20.0
Octanoic acid	10.081	4.6	ng/ul	196299	2	10.787	846614	20.0
Nonanoic acid	11.563	3.5	ng/ul	149613	2	10.787	846614	20.0
1-Nonanamine, N...	14.522	9.8	ng/ul	540528	3	14.640	1103020	20.0
1-Hexadecanamin...	16.375	2.1	ng/ul	141213	4	17.428	1322170	20.0
Hexadecanoic ac...	19.657	3.9	ng/ul	273597	5	21.557	1398650	20.0
Octadecanoic ac...	20.680	3.0	ng/ul	212456	5	21.557	1398650	20.0