

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
 Data File : BP013294.D
 Acq On : 24 Dec 2022 11:52
 Operator : CG/JU
 Sample : N6016-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DBYA7

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-BP120722.M
 Title : SVOA CALIBRATION

Signal : TIC: BP013294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.328	21	24	32	rVB	117888	165219	0.86%	0.110%
2	3.764	95	98	112	rBV	416579	676808	3.54%	0.451%
3	3.864	112	115	125	rVB2	51814	74938	0.39%	0.050%
4	3.987	131	136	143	rVB	114634	177856	0.93%	0.119%
5	4.087	149	153	158	rVB	52895	68418	0.36%	0.046%
6	4.252	178	181	187	rVB7	13153	21178	0.11%	0.014%
7	4.311	187	191	197	rBV	55000	77720	0.41%	0.052%
8	4.464	213	217	223	rVB5	25684	43287	0.23%	0.029%
9	4.652	245	249	253	rVV	32658	47872	0.25%	0.032%
10	4.699	253	257	266	rVB	124199	201069	1.05%	0.134%
11	4.911	287	293	294	rBV6	14927	25803	0.14%	0.017%
12	5.023	306	312	324	rVB3	413120	818097	4.28%	0.545%
13	5.122	325	329	332	rBV3	24216	36564	0.19%	0.024%
14	5.628	410	415	420	rVB2	18269	27542	0.14%	0.018%
15	6.540	565	570	576	rVB3	45516	72395	0.38%	0.048%
16	7.105	658	666	679	rVB	2013238	3287672	17.21%	2.191%
17	7.269	685	694	702	rBV	1656126	2559354	13.40%	1.706%
18	7.469	721	728	736	rBV	2092400	3238880	16.95%	2.159%
19	7.552	738	742	745	rVV4	24812	33454	0.18%	0.022%
20	7.940	801	808	815	rBV	2706047	4183524	21.90%	2.788%
21	8.652	922	929	940	rBV	2403920	3794442	19.86%	2.529%
22	8.769	943	949	958	rVB	147112	239180	1.25%	0.159%
23	9.111	999	1007	1015	rBV	1893419	3105561	16.26%	2.070%
24	9.269	1031	1034	1039	rVB7	15695	22280	0.12%	0.015%
25	9.505	1069	1074	1081	rBV2	63091	102346	0.54%	0.068%
26	9.834	1123	1130	1140	rBV	1586002	2577258	13.49%	1.718%
27	9.993	1150	1157	1162	rBV7	15985	36218	0.19%	0.024%
28	10.058	1164	1168	1173	rVB7	13180	23450	0.12%	0.016%
29	10.193	1184	1191	1196	rVB6	16722	36495	0.19%	0.024%
30	10.375	1214	1222	1239	rBV	2370089	4015721	21.02%	2.676%
31	10.752	1277	1286	1293	rBV	3374161	5850568	30.62%	3.899%
32	10.893	1303	1310	1332	rVB	1904509	3280780	17.17%	2.187%
33	11.299	1371	1379	1384	rBV	12391	24322	0.13%	0.016%
34	11.546	1415	1421	1426	rBV10	16350	34874	0.18%	0.023%
35	12.157	1520	1525	1532	rVB2	24683	38747	0.20%	0.026%
36	12.340	1550	1556	1562	rVB	42598	75564	0.40%	0.050%

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37	12.410	1562	1568	1573	rBV9	9009	19461	0.10%	0.013%
38	13.104	1681	1686	1691	rBV4	29455	44308	0.23%	0.030%
39	13.399	1726	1736	1744	rBV2	63550	116135	0.61%	0.077%
40	13.904	1817	1822	1829	rBV9	23074	38615	0.20%	0.026%

41	13.993	1830	1837	1845	rBV	3947336	5255674	27.51%	3.503%
42	14.098	1852	1855	1860	rVB6	13699	22926	0.12%	0.015%
43	14.281	1871	1886	1904	rBV	4271900	6403740	33.52%	4.268%
44	14.469	1914	1918	1923	rVB2	34418	46521	0.24%	0.031%
45	14.587	1931	1938	1946	rBV	4594168	6641267	34.76%	4.426%

46	14.787	1965	1972	1989	rBV	971864	1730096	9.06%	1.153%
47	14.998	2003	2008	2018	rVB3	90647	179911	0.94%	0.120%
48	15.369	2066	2071	2074	rBV6	12569	21776	0.11%	0.015%
49	15.422	2076	2080	2083	rVB5	21876	28291	0.15%	0.019%
50	15.581	2100	2107	2113	rBV	5183120	7367788	38.57%	4.911%

51	15.634	2113	2116	2121	rVB	23233	35546	0.19%	0.024%
52	15.698	2121	2127	2137	rBV	891381	1213057	6.35%	0.808%
53	15.822	2143	2148	2154	rVB4	28898	51102	0.27%	0.034%
54	15.945	2164	2169	2179	rVB	136899	224730	1.18%	0.150%
55	16.081	2189	2192	2196	rVB4	14733	19684	0.10%	0.013%

56	16.287	2224	2227	2230	rBV4	19360	26219	0.14%	0.017%
57	16.510	2262	2265	2272	rVB8	19895	29310	0.15%	0.020%
58	16.740	2298	2304	2311	rBV4	100480	149148	0.78%	0.099%
59	17.092	2359	2364	2367	rBV6	21831	35153	0.18%	0.023%
60	17.228	2382	2387	2395	rBV5	25832	53945	0.28%	0.036%

61	17.345	2400	2407	2412	rVV	4764946	6777805	35.48%	4.517%
62	17.387	2412	2414	2418	rVV	154502	188211	0.99%	0.125%
63	17.445	2418	2424	2436	rVV	4932680	7087136	37.10%	4.724%
64	17.534	2436	2439	2446	rVB8	31782	56415	0.30%	0.038%
65	17.728	2468	2472	2473	rBV4	19964	24963	0.13%	0.017%

66	18.004	2515	2519	2523	rVB5	34982	40342	0.21%	0.027%
67	18.098	2532	2535	2539	rBV6	25849	38027	0.20%	0.025%
68	18.157	2541	2545	2549	rBV6	34630	44992	0.24%	0.030%
69	18.216	2550	2555	2560	rBV	720376	954680	5.00%	0.636%
70	18.339	2572	2576	2581	rVB3	47865	73594	0.39%	0.049%

71	18.551	2608	2612	2620	rBV2	97953	155976	0.82%	0.104%
72	18.628	2621	2625	2631	rVB	191012	220429	1.15%	0.147%
73	18.692	2633	2636	2639	rVB3	31233	40782	0.21%	0.027%
74	19.251	2728	2731	2736	rVB4	102729	144686	0.76%	0.096%
75	19.351	2738	2748	2754	rBV2	395979	748723	3.92%	0.499%

76	19.445	2760	2764	2769	rBV	329701	453693	2.37%	0.302%
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77	19.681	2798	2804	2815	rVB	7200198	9859491	51.61%	6.571%
78	20.186	2887	2890	2897	rVB3	232738	362777	1.90%	0.242%
79	20.281	2904	2906	2910	rVB	107884	118961	0.62%	0.079%
80	21.128	3046	3050	3059	rBV2	1216230	1954081	10.23%	1.302%
81	21.328	3082	3084	3089	rVB	241152	230248	1.21%	0.153%
82	21.439	3096	3103	3107	rBV	6300550	9024615	47.24%	6.015%
83	21.475	3107	3109	3115	rVB	579528	687201	3.60%	0.458%
84	22.339	3251	3256	3264	rVB	1952884	2776224	14.53%	1.850%
85	23.763	3491	3498	3512	rVB2	4994801	11203445	58.64%	7.467%
86	23.922	3518	3525	3533	rBV2	4456377	8816492	46.15%	5.876%
87	28.510	4295	4305	4321	rVB3	5102785	19104593	100.00%	12.733%

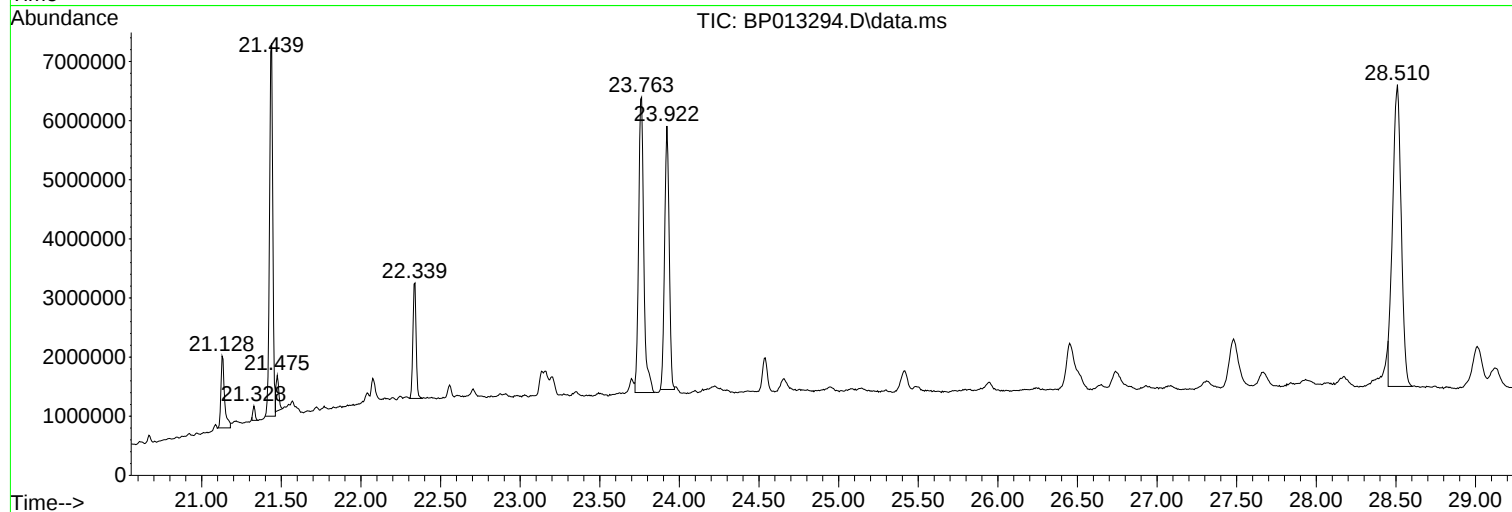
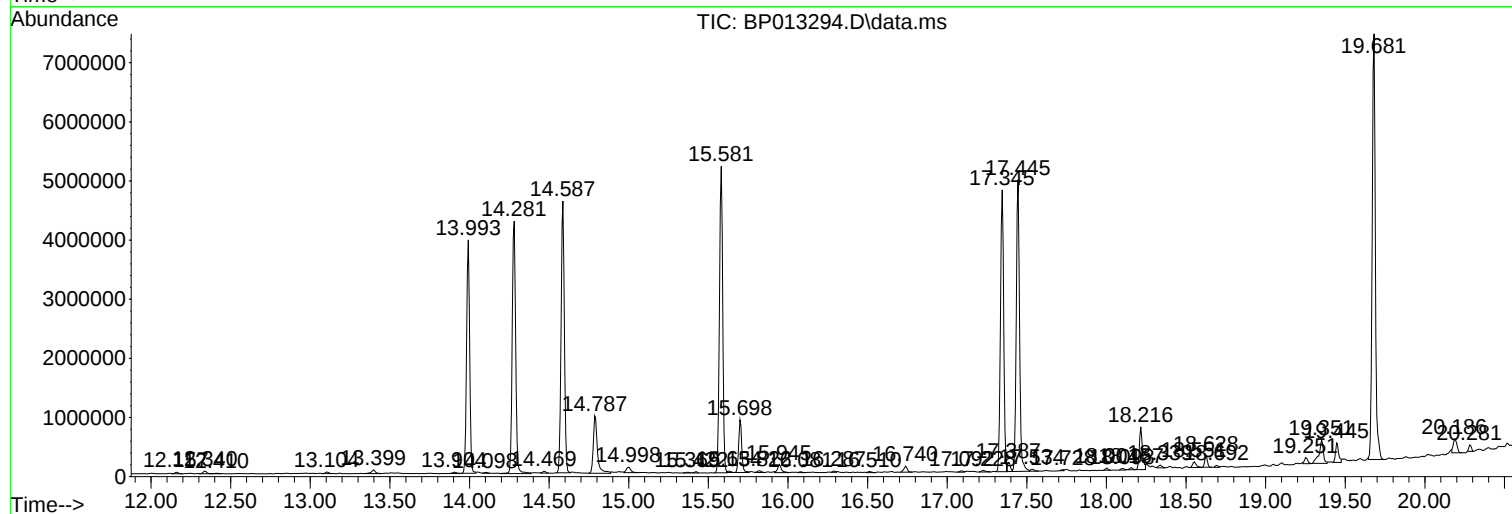
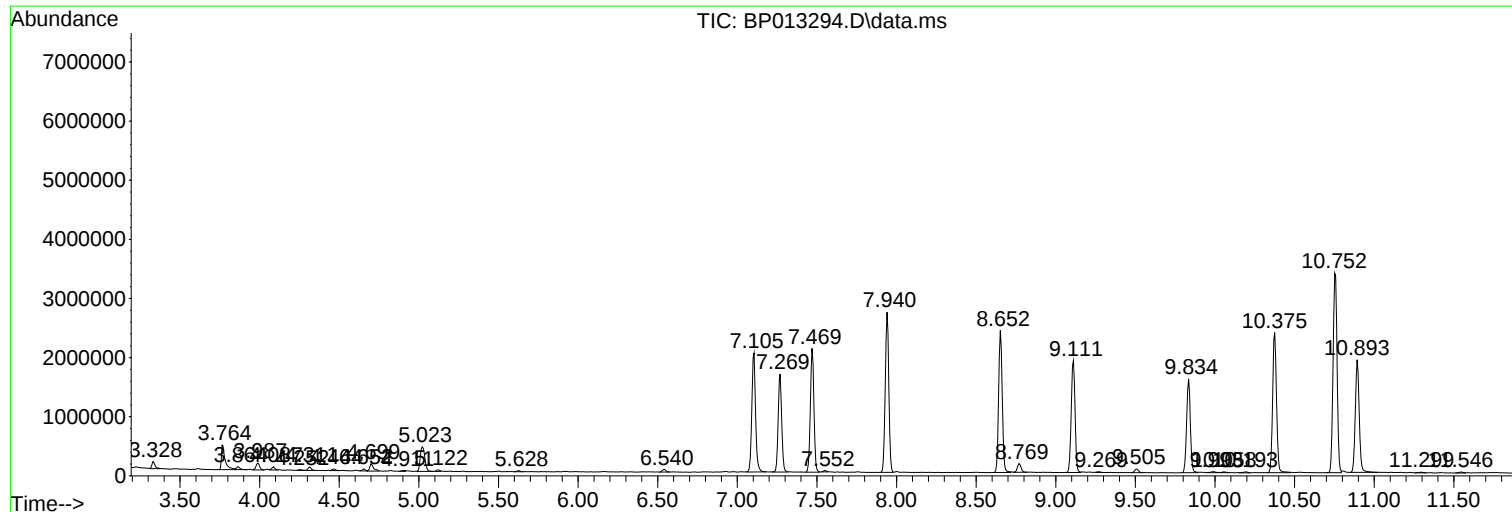
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



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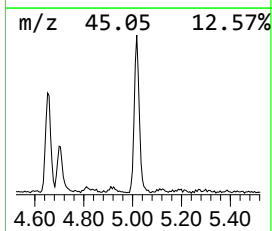
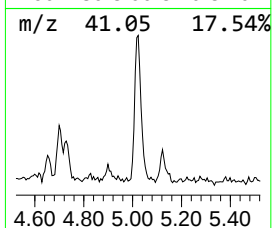
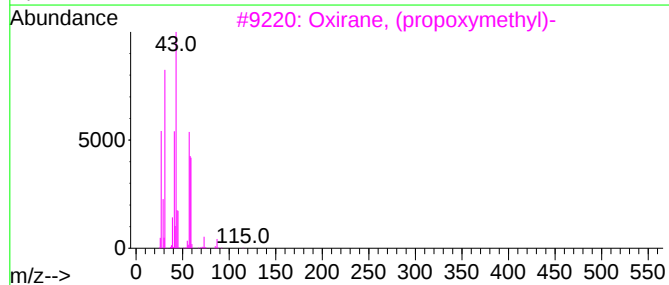
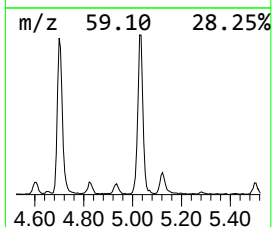
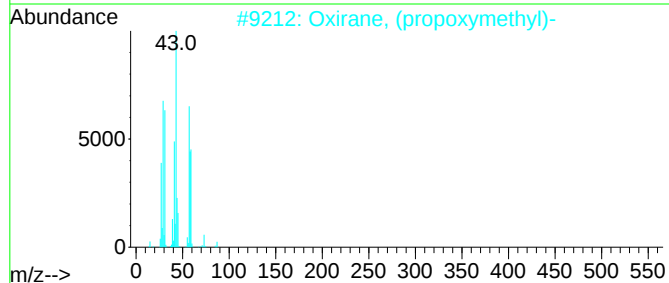
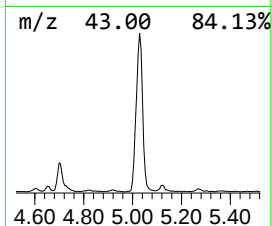
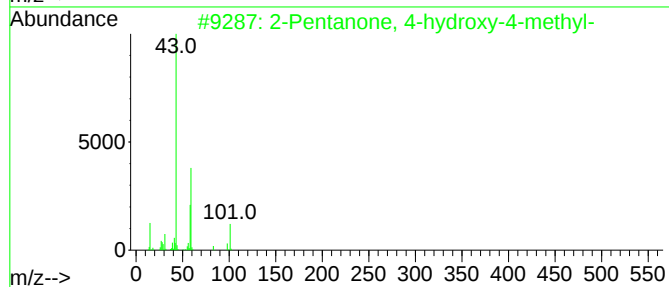
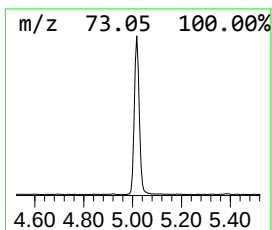
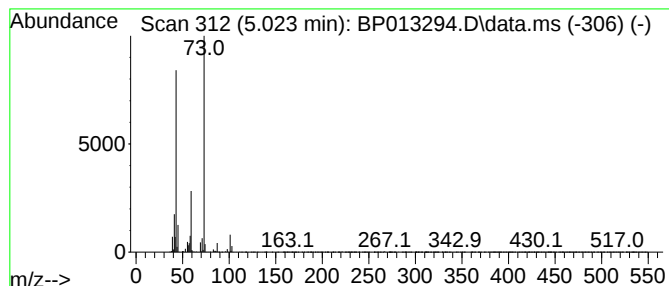
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.023	3.91 ng/ul	818097	1,4-Dichlorobenzene-d4	7.940

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32		
2	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	28		
3	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	23		
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	17		
5	Methyl glyoxal	72	C3H4O2	000078-98-8	12		



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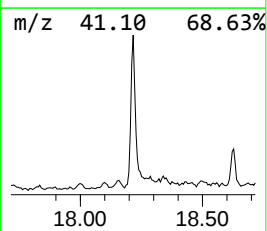
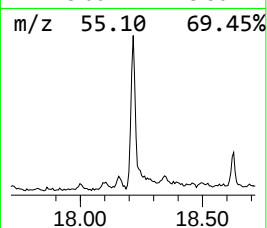
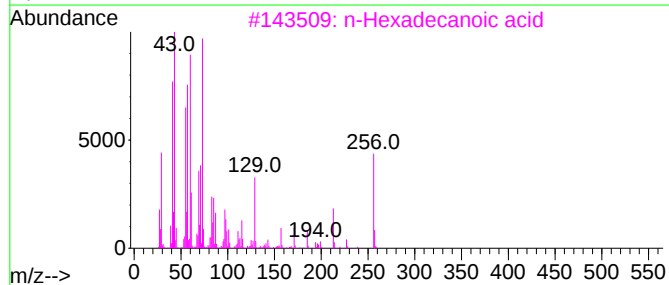
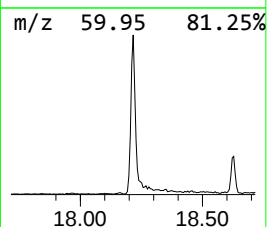
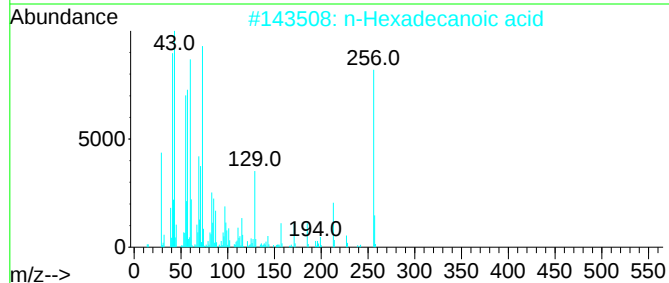
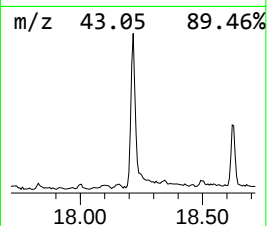
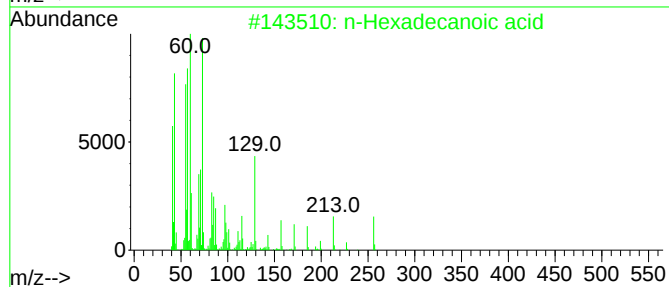
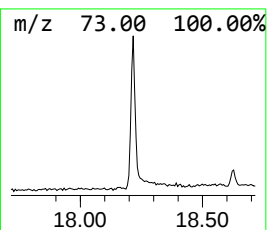
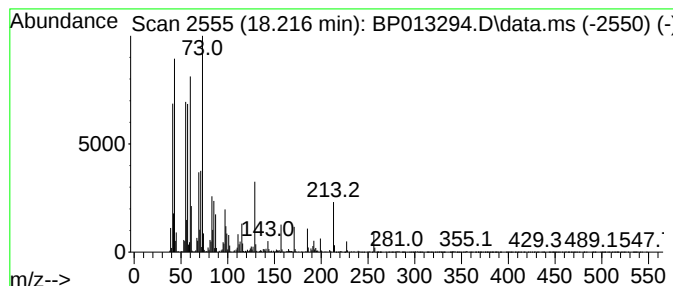
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	2.82 ng/ul	954680	Phenanthrene-d10	17.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	93



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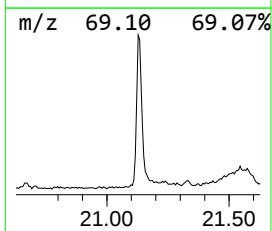
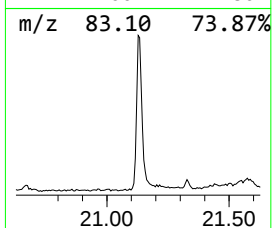
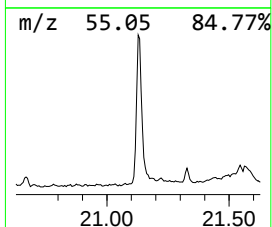
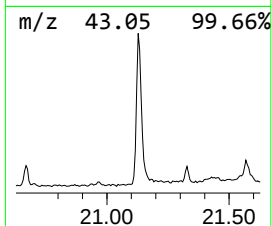
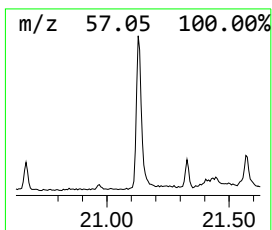
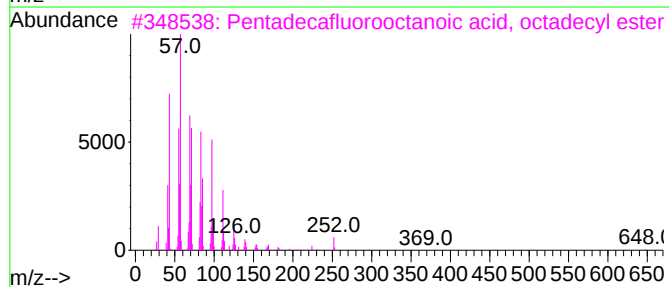
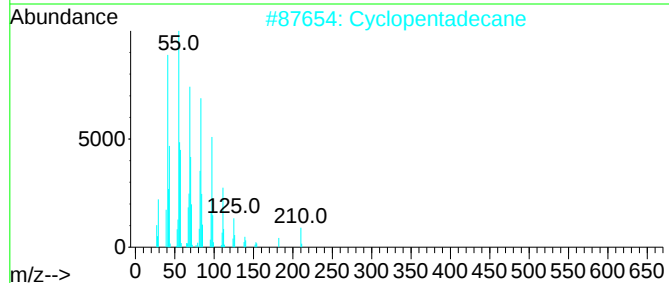
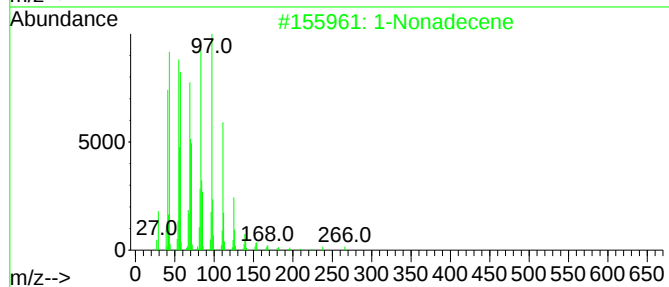
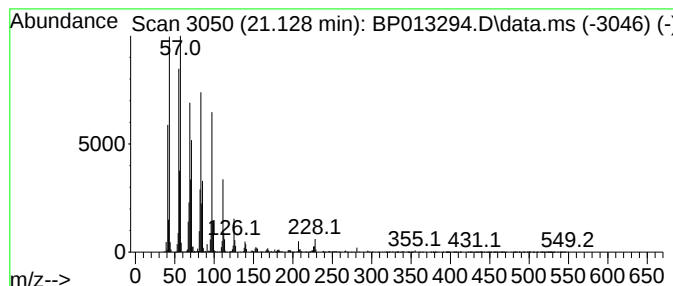
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	4.33 ng/ul	1954080	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	97
2	Cyclopentadecane			210	C15H30	000295-48-7	96
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94
4	Octacosanol			410	C28H58O	000557-61-9	94
5	1-Octadecene			252	C18H36	000112-88-9	93



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ClientSampleId :
DBYA7

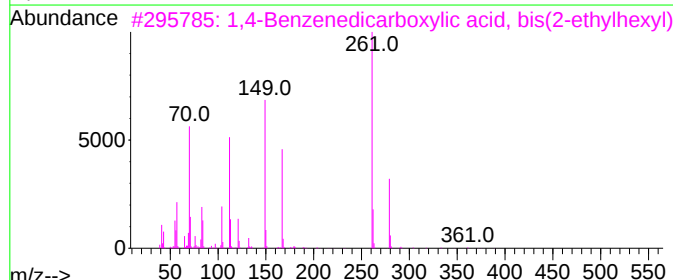
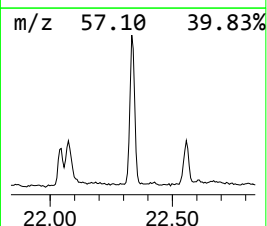
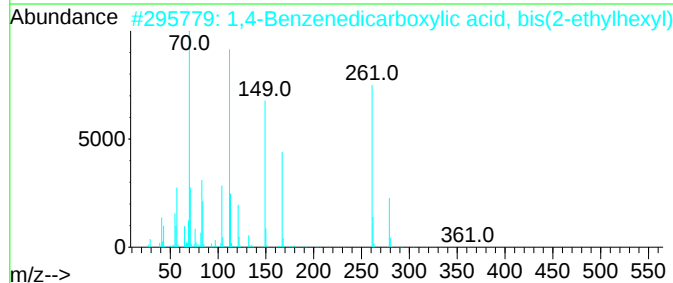
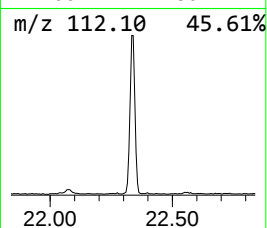
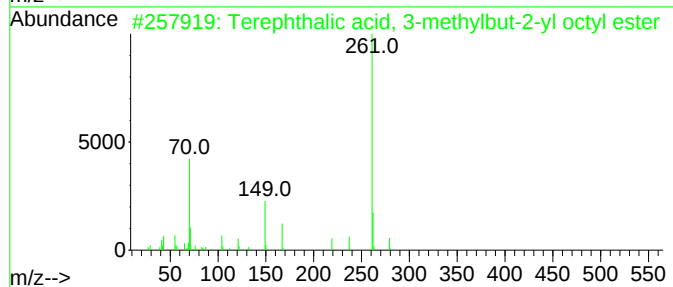
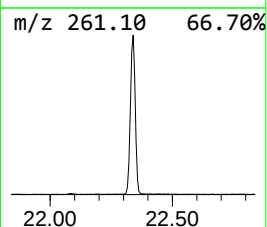
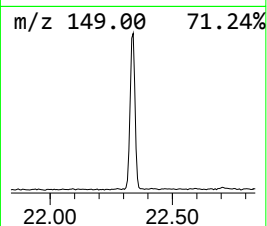
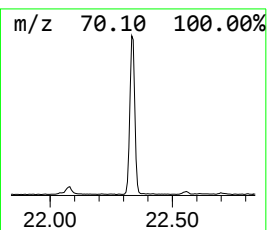
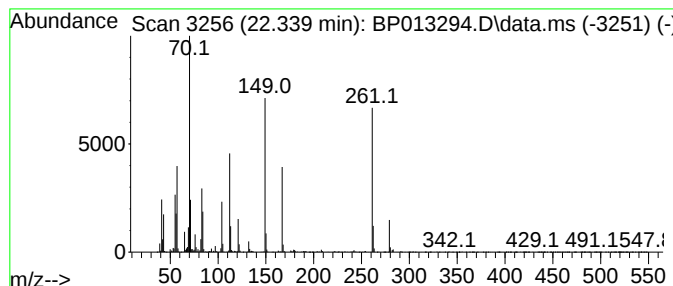
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Terephthalic acid, 3-methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.339	6.15 ng/ul	2776220	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
4			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	58
5			Isophthalic acid, 3-methylbut-2...	348	C21H32O4	1000344-72-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013294.D
Acq On : 24 Dec 2022 11:52
Operator : CG/JU
Sample : N6016-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYA7

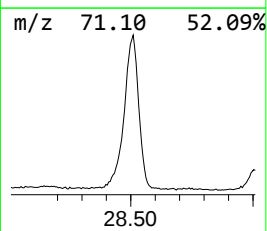
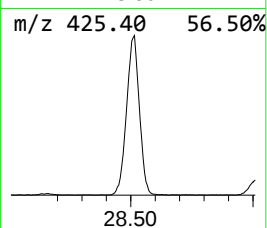
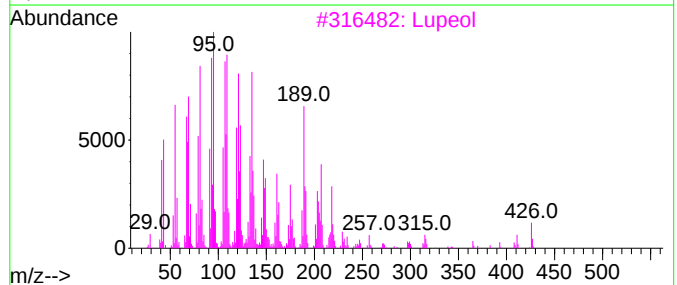
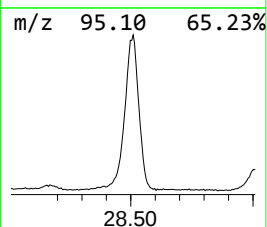
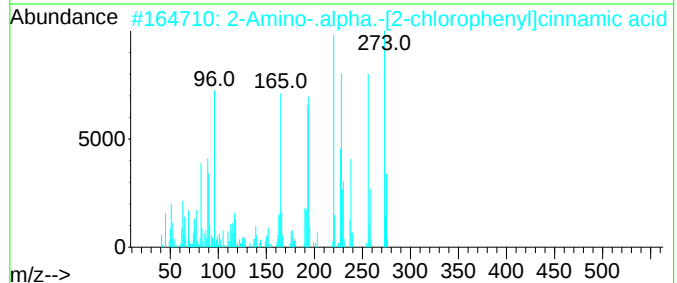
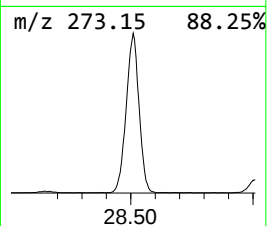
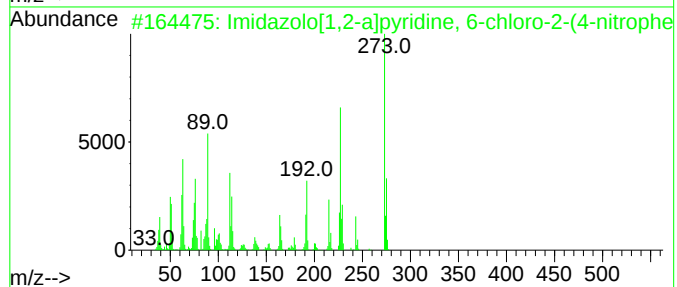
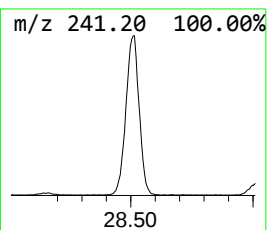
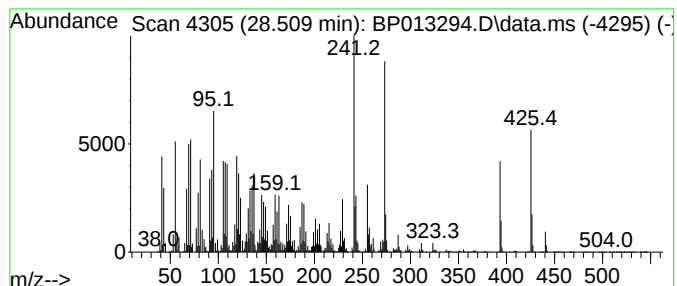
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Imidazolo[1,2-a]pyridine, 6... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.509	43.34 ng/ul	19104600	Perylene-d12	23.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	90
2			2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	53
3			Lupeol	426	C30H50O	000545-47-1	52
4			1-Naphthalenepropanol, .alpha.-e...	306	C20H34O2	001908-44-7	22
5			2-(Phenylmethyl)phenol, tert-but...	298	C19H26OSi	1417315-87-7	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122422\
Data File : BP013294.D
Acq On : 24 Dec 2022 11:52
Operator : CG/JU
Sample : N6016-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBYA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
2-Pentanone, 4-...	5.023	3.9	ng/ul	818097	1	7.940	4183520	20.0
n-Hexadecanoic ...	18.216	2.8	ng/ul	954680	4	17.345	6777810	20.0
(DEL) Alkane: S...	21.128	4.3	ng/ul	1954080	5	21.439	9024620	20.0
Terephthalic ac...	22.339	6.2	ng/ul	2776220	5	21.439	9024620	20.0
Imidazolo[1,2-a...	28.509	43.3	ng/ul	19104600	6	23.922	8816490	20.0