

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111924\
 Data File : BP023293.D
 Acq On : 21 Nov 2024 20:48
 Operator : RC/JU
 Sample : P4881-05
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0TF5

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-BP110924.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP023293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.058	8	12	17	rBV3	7424	11938	0.44%	0.040%
2	3.134	21	25	33	rVB2	15751	23785	0.88%	0.080%
3	3.852	143	147	151	rBV2	5235	7135	0.26%	0.024%
4	4.275	217	219	226	rVB3	3560	5113	0.19%	0.017%
5	6.011	510	514	519	rBV8	1610	2908	0.11%	0.010%
6	6.269	553	558	564	rBV2	10667	17115	0.63%	0.057%
7	6.522	596	601	606	rBV5	6381	10061	0.37%	0.034%
8	6.699	625	631	633	rBV7	2498	3566	0.13%	0.012%
9	6.764	636	642	661	rVV	221049	461111	17.08%	1.549%
10	6.911	661	667	678	rVV	175976	317328	11.75%	1.066%
11	7.005	678	683	691	rVV	16536	31097	1.15%	0.104%
12	7.111	694	701	720	rVB	260247	438414	16.24%	1.473%
13	7.452	753	759	763	rVB	19917	29172	1.08%	0.098%
14	7.552	770	776	788	rBV	322691	583990	21.63%	1.962%
15	7.769	809	813	819	rVB8	5380	8625	0.32%	0.029%
16	8.275	891	899	920	rBV	242526	562730	20.84%	1.890%
17	8.705	965	972	991	rBV	228579	449327	16.64%	1.509%
18	8.869	994	1000	1003	rBV7	2154	2749	0.10%	0.009%
19	9.093	1032	1038	1042	rBV5	5491	9906	0.37%	0.033%
20	9.269	1064	1068	1077	rBV4	11518	25219	0.93%	0.085%
21	9.422	1087	1094	1107	rBV	190041	385472	14.28%	1.295%
22	9.963	1180	1186	1208	rBV	240628	598950	22.18%	2.012%
23	10.305	1236	1244	1253	rBV	465565	754482	27.94%	2.534%
24	10.469	1264	1272	1294	rBV	128668	336188	12.45%	1.129%
25	10.905	1338	1346	1349	rBV8	5206	10267	0.38%	0.034%
26	11.563	1454	1458	1462	rVB5	2411	3267	0.12%	0.011%
27	11.722	1481	1485	1492	rVB9	2275	3891	0.14%	0.013%
28	11.922	1512	1519	1526	rBV4	3915	8559	0.32%	0.029%
29	12.510	1611	1619	1630	rBV8	15458	31419	1.16%	0.106%
30	12.599	1630	1634	1637	rVB5	1900	2899	0.11%	0.010%
31	12.693	1647	1650	1654	rBV6	1457	2745	0.10%	0.009%
32	12.881	1677	1682	1685	rBV2	23404	37830	1.40%	0.127%
33	13.034	1702	1708	1716	rVB3	38023	66763	2.47%	0.224%
34	13.157	1725	1729	1734	rBV7	2801	4897	0.18%	0.016%
35	13.434	1763	1776	1781	rBV7	9758	25314	0.94%	0.085%
36	13.487	1781	1785	1792	rVV10	7451	16460	0.61%	0.055%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0.1 % of largest Peak
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37	13.581	1794	1801	1814	rVV	664564	943908	34.96%	3.171%
38	13.693	1816	1820	1823	rVB6	2083	3368	0.12%	0.011%
39	13.775	1831	1834	1837	rBV5	2472	2780	0.10%	0.009%
40	13.869	1841	1850	1858	rBV2	592484	1019664	37.76%	3.425%
41	14.004	1867	1873	1878	rBV4	28135	49132	1.82%	0.165%
42	14.057	1878	1882	1887	rBV7	5095	9297	0.34%	0.031%
43	14.134	1887	1895	1898	rBV	183686	286146	10.60%	0.961%
44	14.181	1898	1903	1910	rVV	688909	1077881	39.92%	3.621%
45	14.240	1910	1913	1920	rVB	42927	59008	2.19%	0.198%
46	14.434	1936	1946	1949	rBV2	55219	96412	3.57%	0.324%
47	14.475	1949	1953	1955	rVV2	97216	150102	5.56%	0.504%
48	14.504	1956	1958	1972	rVV3	105031	226386	8.38%	0.760%
49	14.610	1972	1976	1979	rVB6	7097	11376	0.42%	0.038%
50	14.710	1989	1993	2000	rVB4	9274	19084	0.71%	0.064%
51	14.804	2004	2009	2012	rVB7	2703	4992	0.18%	0.017%
52	14.922	2025	2029	2032	rVB6	3694	4723	0.17%	0.016%
53	15.093	2053	2058	2067	rVB6	11017	21380	0.79%	0.072%
54	15.204	2069	2077	2087	rBV	834622	1349056	49.96%	4.531%
55	15.351	2097	2102	2113	rBV	188201	341014	12.63%	1.145%
56	15.575	2127	2140	2150	rBV	272661	474022	17.55%	1.592%
57	15.681	2151	2158	2165	rVB2	36518	62711	2.32%	0.211%
58	15.775	2169	2174	2181	rBV6	14725	26483	0.98%	0.089%
59	15.857	2181	2188	2196	rVB6	9432	21194	0.78%	0.071%
60	15.940	2196	2202	2207	rBV6	7879	14666	0.54%	0.049%
61	16.022	2211	2216	2221	rBV2	48311	79596	2.95%	0.267%
62	16.145	2232	2237	2244	rVB4	9873	19284	0.71%	0.065%
63	16.404	2277	2281	2286	rBV7	6405	11497	0.43%	0.039%
64	16.728	2333	2336	2339	rBV5	2710	3543	0.13%	0.012%
65	16.904	2362	2366	2373	rBV8	11864	18459	0.68%	0.062%
66	16.998	2374	2382	2393	rVV	965223	1467744	54.35%	4.930%
67	17.098	2393	2399	2411	rVV	1246493	1574748	58.32%	5.289%
68	17.192	2412	2415	2419	rVB5	8934	13191	0.49%	0.044%
69	17.410	2450	2452	2455	rBV4	2264	3241	0.12%	0.011%
70	17.692	2492	2500	2504	rBV4	6727	16534	0.61%	0.056%
71	17.816	2515	2521	2526	rBV8	12863	26144	0.97%	0.088%
72	17.869	2526	2530	2535	rBV5	15811	25105	0.93%	0.084%
73	17.934	2535	2541	2553	rBV	527102	766869	28.40%	2.576%
74	18.234	2588	2592	2600	rVB7	32279	58548	2.17%	0.197%
75	18.381	2615	2617	2623	rVB7	8939	15193	0.56%	0.051%
76	18.645	2659	2662	2663	rBV3	8286	9438	0.35%	0.032%

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77	18.804	2682	2689	2695	rBV8	40018	137023	5.07%	0.460%
78	19.022	2723	2726	2730	rVB6	26454	38523	1.43%	0.129%
79	19.151	2738	2748	2762	rBV	1041146	1896248	70.22%	6.369%
80	19.281	2765	2770	2787	rVB2	224826	420330	15.57%	1.412%
81	19.481	2798	2804	2812	rVV	1231579	1915891	70.95%	6.435%
82	19.545	2812	2815	2820	rVB4	20021	26556	0.98%	0.089%
83	20.063	2900	2903	2911	rVB7	37622	74123	2.74%	0.249%
84	20.910	3042	3047	3058	rVB	2183550	2700298	100.00%	9.070%
85	21.122	3077	3083	3093	rBV4	126789	412779	15.29%	1.386%
86	21.439	3131	3137	3148	rBV2	1204595	2031755	75.24%	6.824%
87	24.433	3638	3646	3658	rVB	861313	2206122	81.70%	7.410%
88	24.651	3675	3683	3705	rVB	763560	2237232	82.85%	7.515%

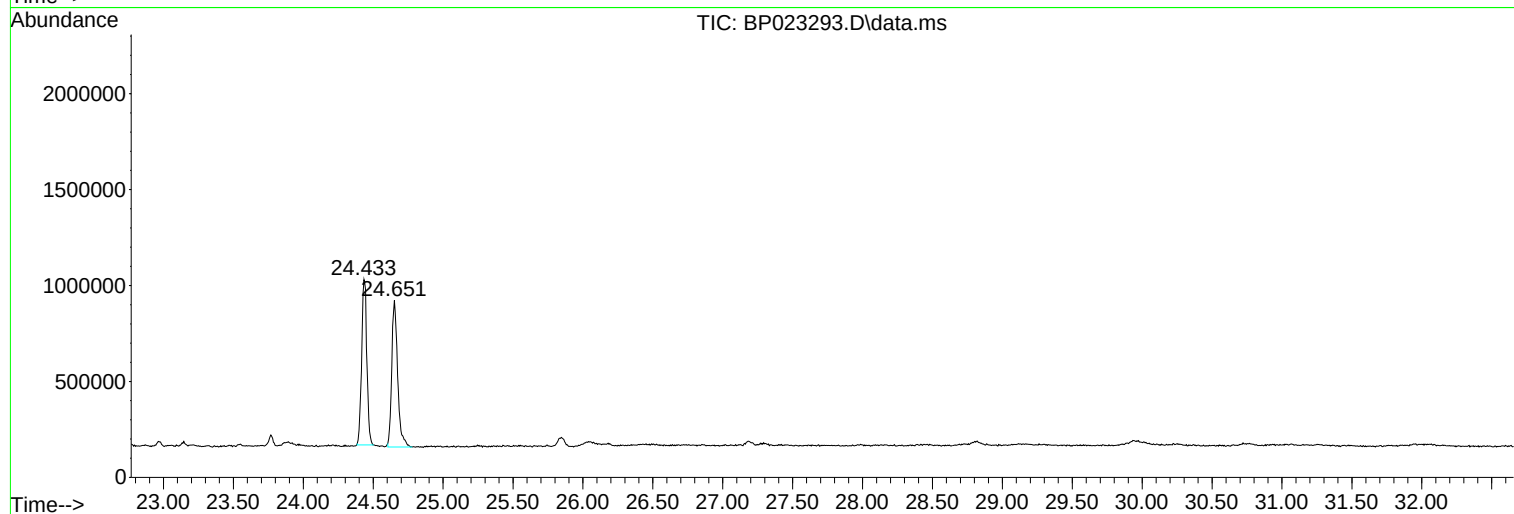
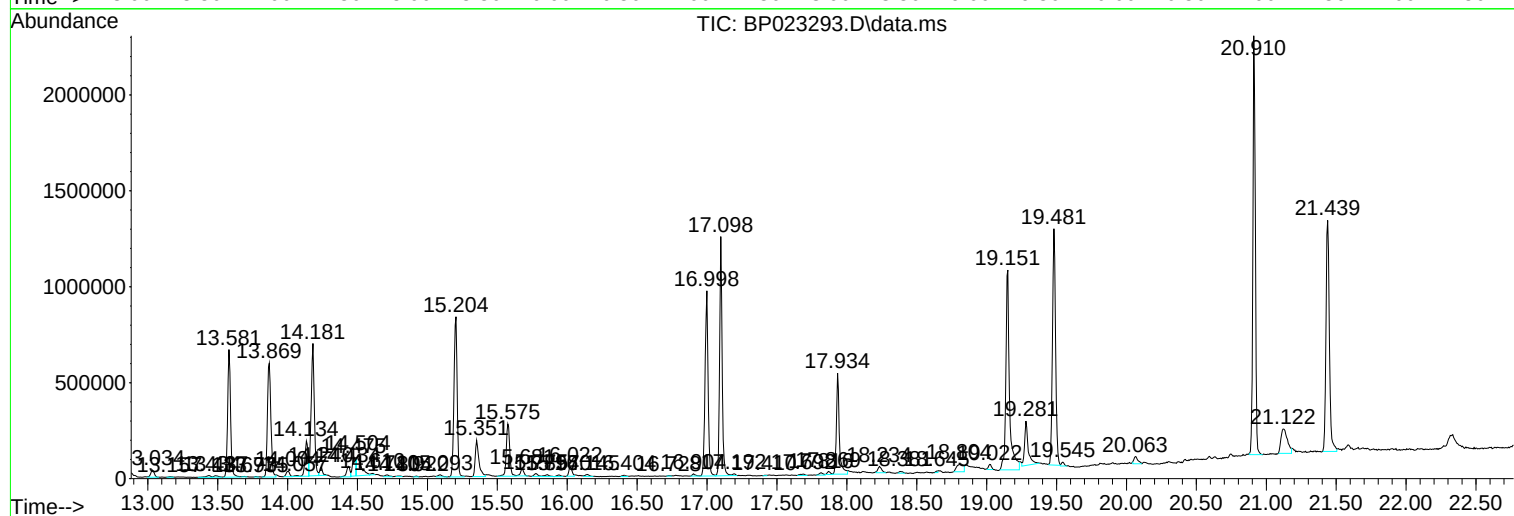
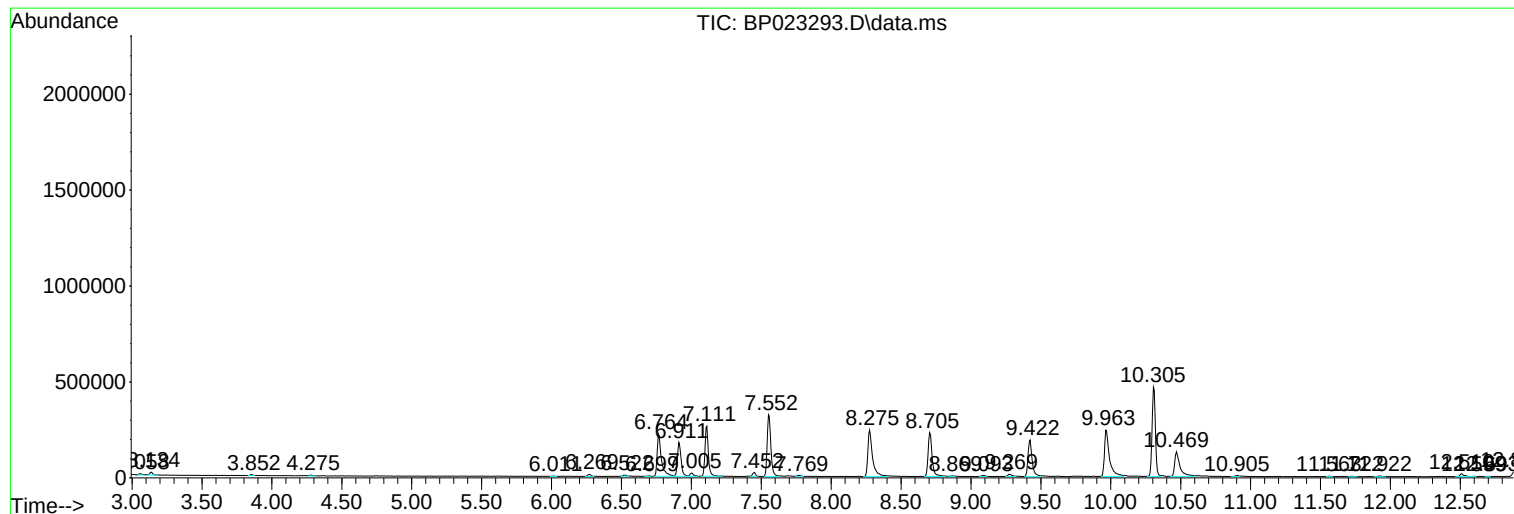
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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



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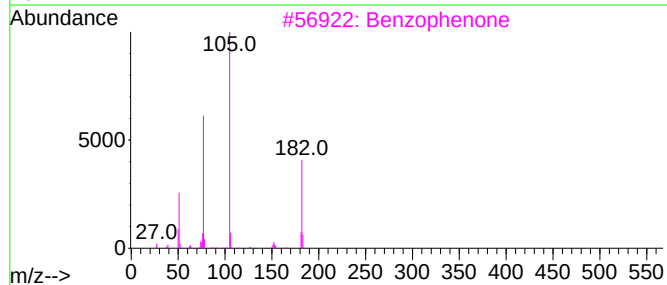
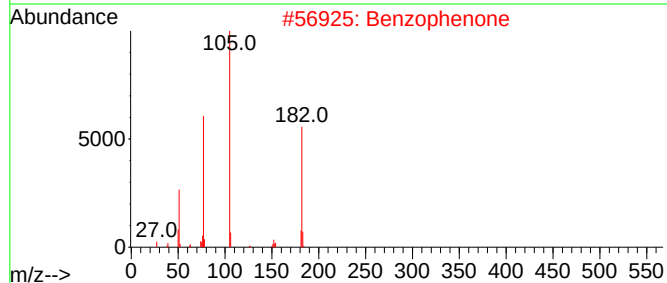
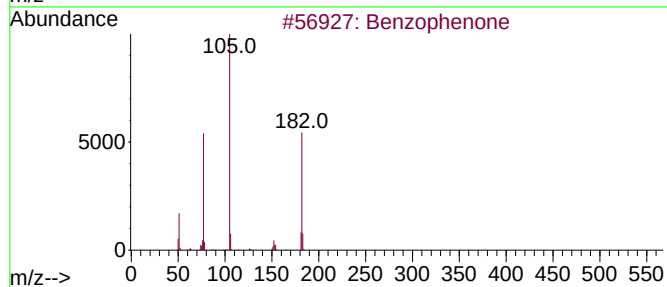
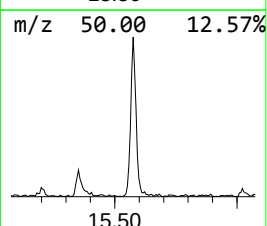
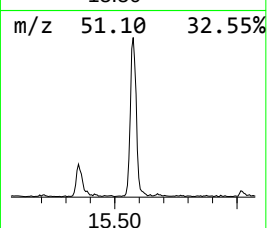
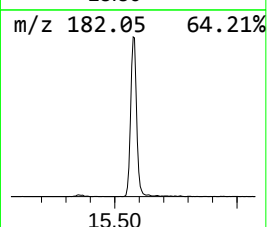
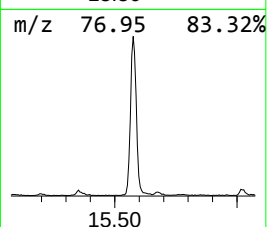
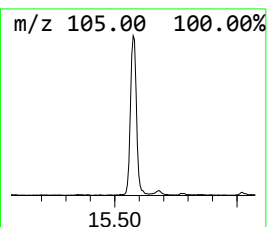
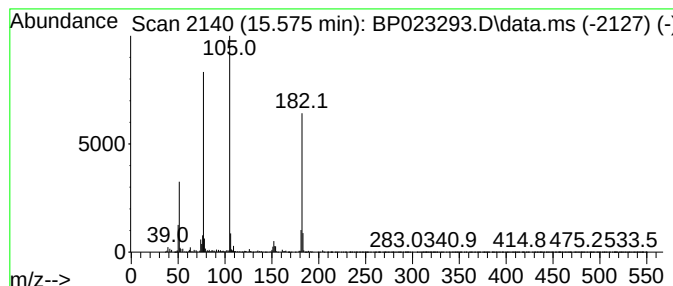
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.575	8.80 ng/ul	474022	Acenaphthene-d10	14.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	94
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	78



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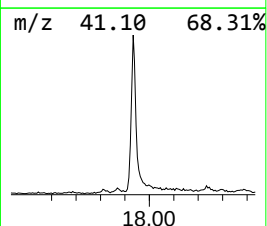
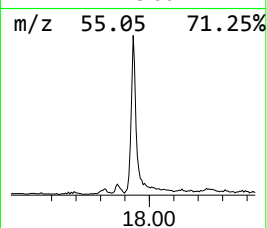
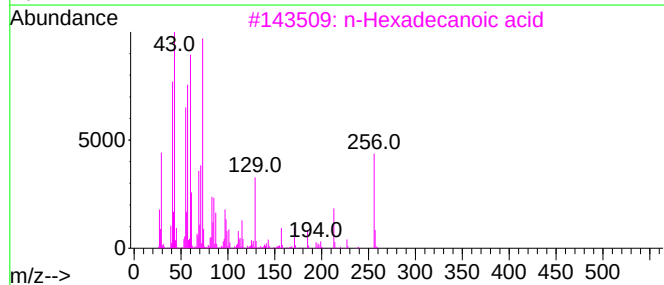
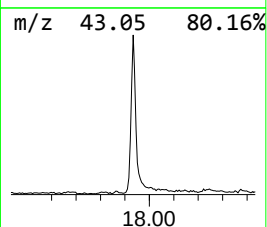
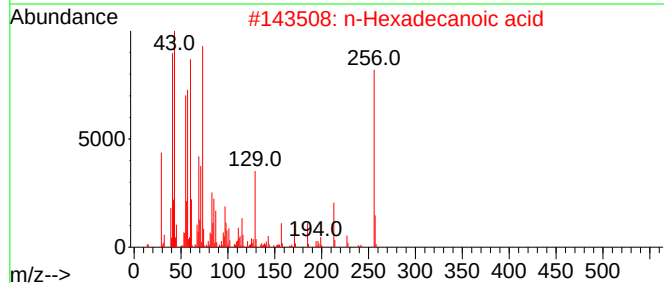
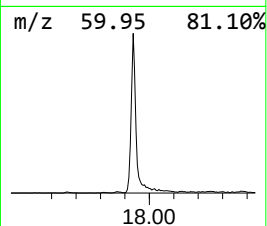
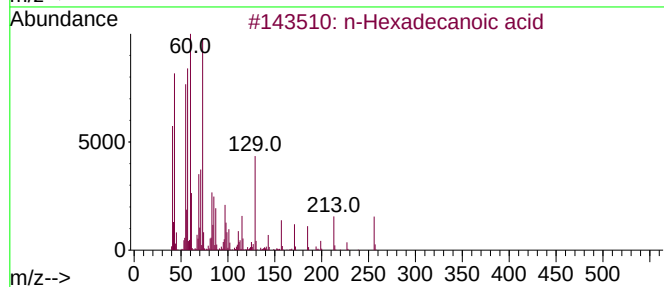
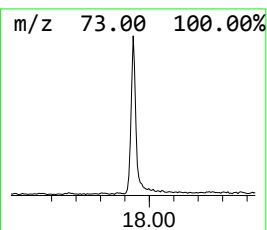
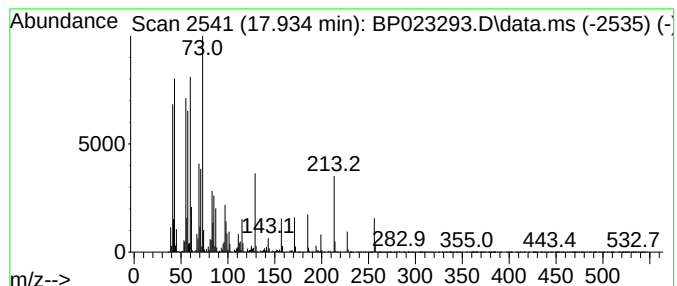
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.934	10.45 ng/ul	766869	Phenanthrene-d10	16.998

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	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5			Tridecanoic acid	214	C13H26O2	000638-53-9	94



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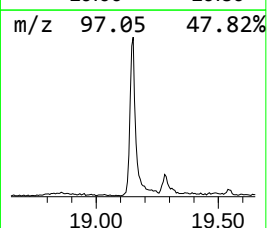
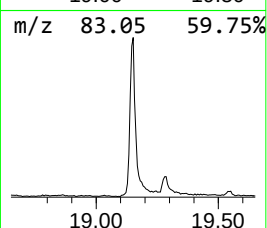
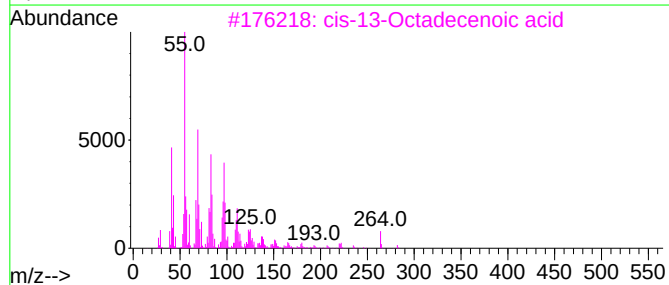
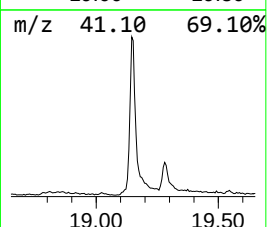
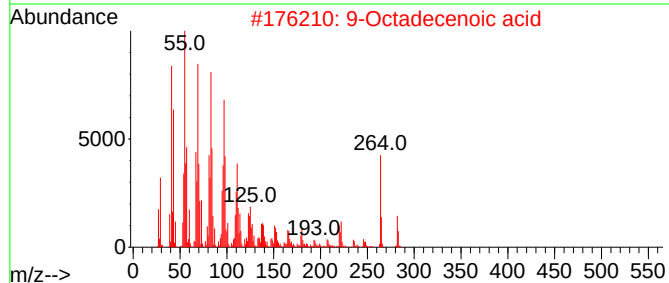
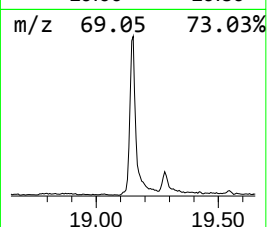
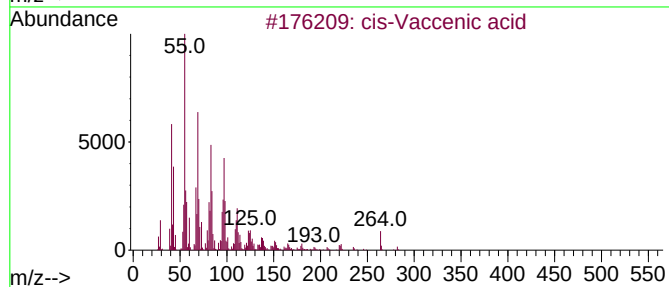
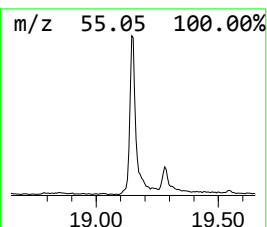
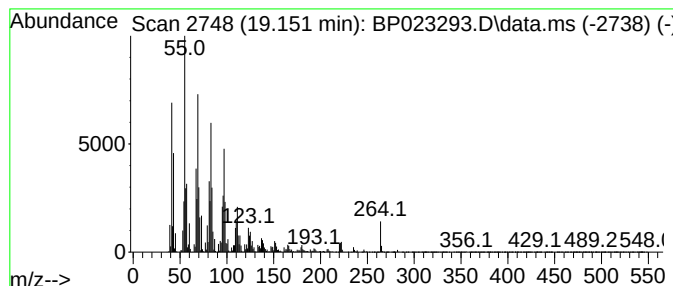
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 cis-Vaccenic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.151	25.84 ng/ul	1896250	Phenanthrene-d10	16.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	94
2			9-Octadecenoic acid	282	C18H34O2	002027-47-6	91
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	90
4			Palmitoleic acid	254	C16H30O2	000373-49-9	87
5			6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	87



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C0TF5

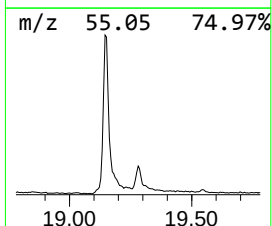
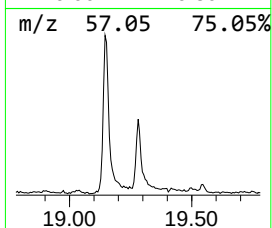
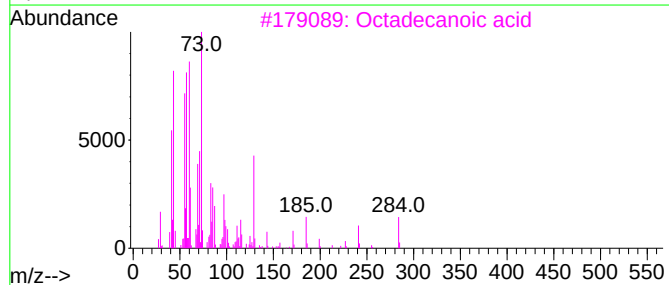
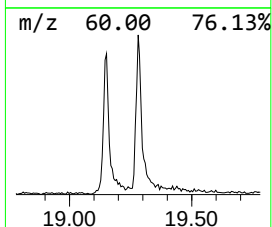
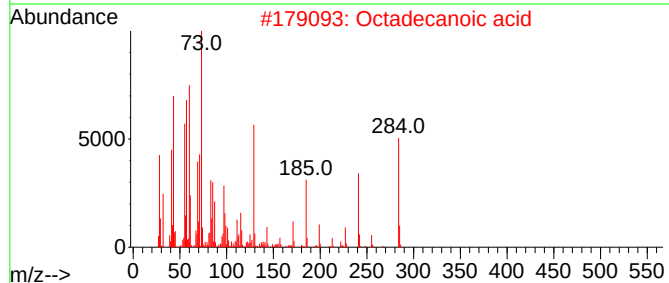
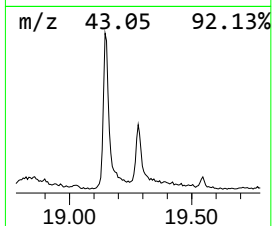
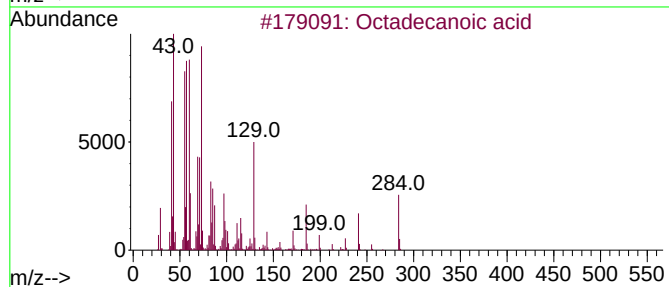
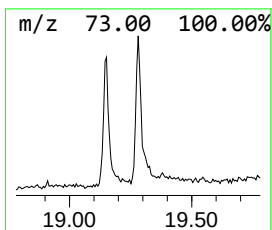
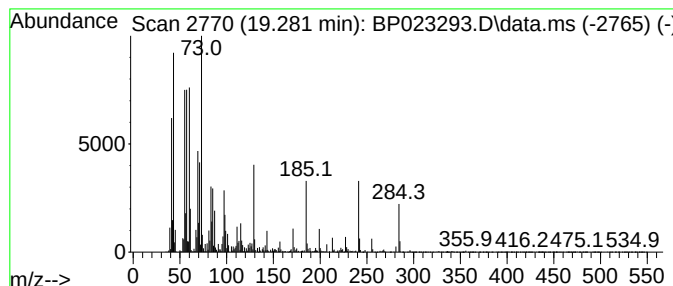
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.281	4.14 ng/ul	420330	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	99
3			Octadecanoic acid	284	C18H36O2	000057-11-4	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111924\
Data File : BP023293.D
Acq On : 21 Nov 2024 20:48
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0TF5

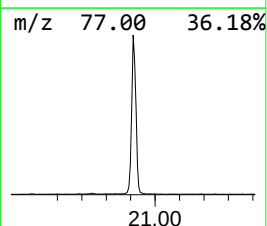
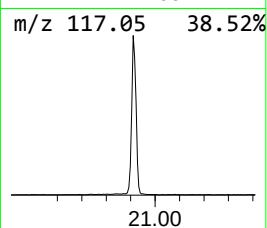
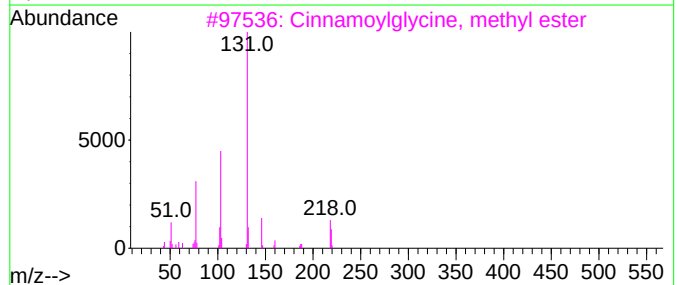
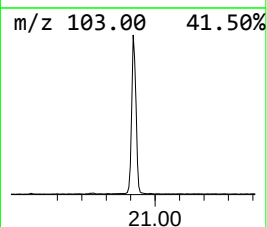
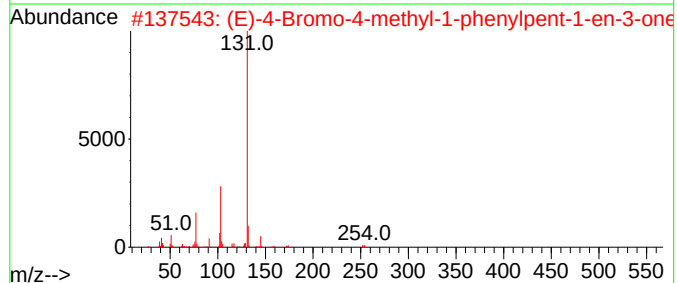
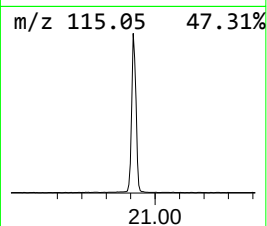
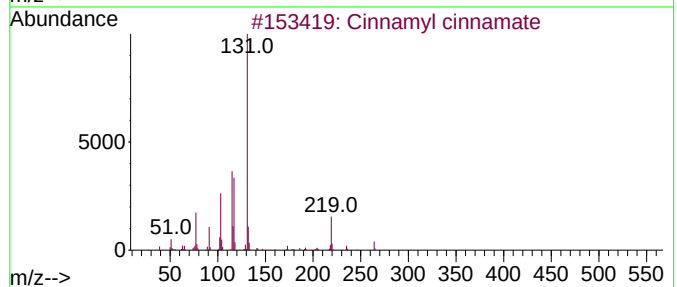
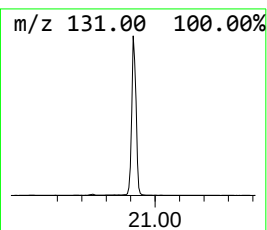
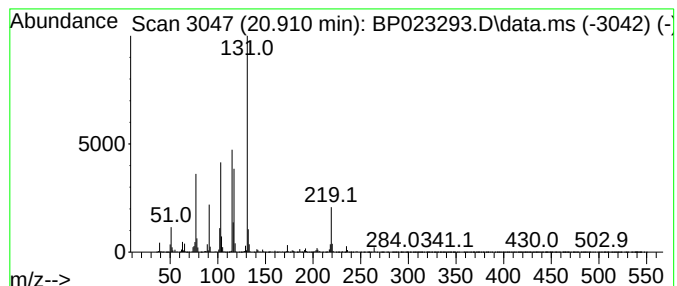
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Cinnamyl cinnamate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.910	26.58 ng/ul	2700300	Chrysene-d12	21.439

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	87
2			(E)-4-Bromo-4-methyl-1-phenylpen...	252	C12H13BrO	1000443-02-8	47
3			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	47
4			Allyl cinnamate	188	C12H12O2	001866-31-5	43
5			p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111924\
Data File : BP023293.D
Acq On : 21 Nov 2024 20:48
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0TF5

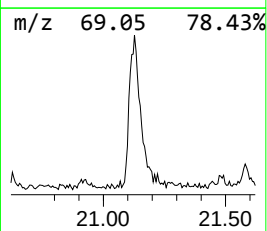
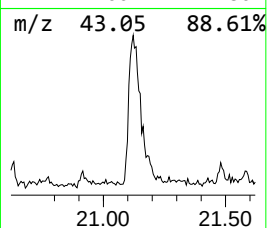
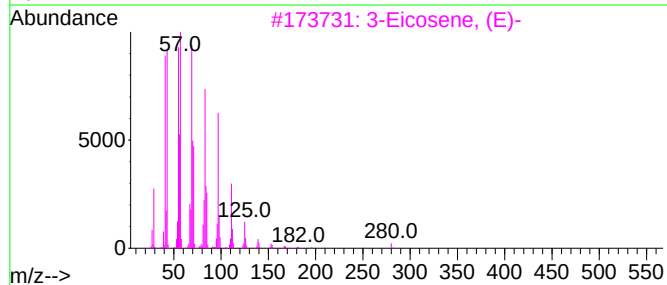
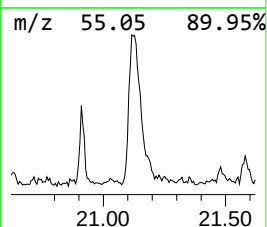
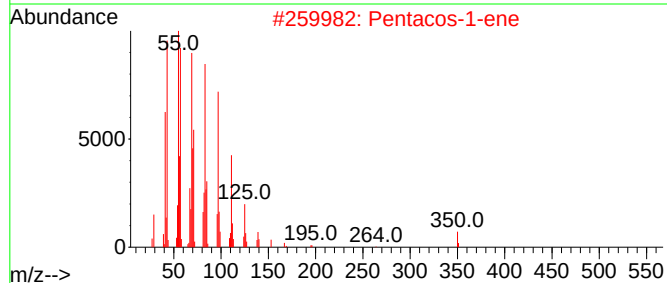
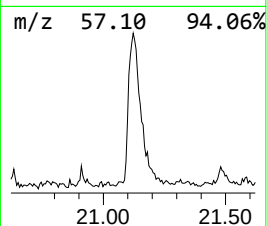
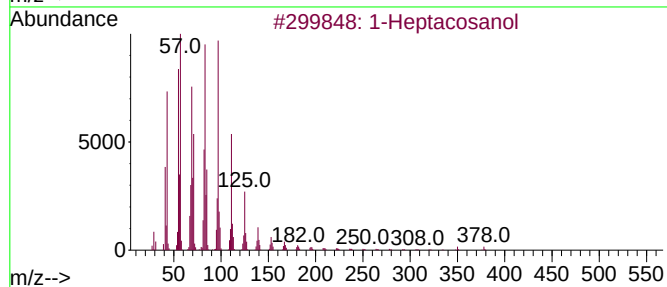
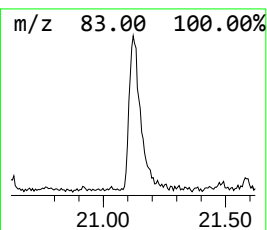
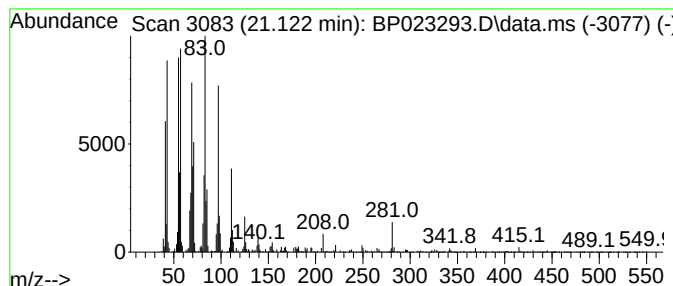
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.122	4.06 ng/ul	412779	Chrysene-d12	21.439

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heptacosanol	396	C27H56O	002004-39-9	94
2		Pentacos-1-ene	350	C25H50	016980-85-1	94
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111924\
Data File : BP023293.D
Acq On : 21 Nov 2024 20:48
Operator : RC/JU
Sample : P4881-05
Misc :
ALS Vial : 52 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0TF5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.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
Benzophenone	15.575	8.8	ng/ul	474022	3	14.181	1077880	20.0
n-Hexadecanoic ...	17.934	10.4	ng/ul	766869	4	16.998	1467740	20.0
cis-Vaccenic acid	19.151	25.8	ng/ul	1896250	4	16.998	1467740	20.0
Octadecanoic acid	19.281	4.1	ng/ul	420330	5	21.439	2031760	20.0
Cinnamyl cinnamate	20.910	26.6	ng/ul	2700300	5	21.439	2031760	20.0
1-Heptacosanol	21.122	4.1	ng/ul	412779	5	21.439	2031760	20.0