

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
 Data File : BP022174.D
 Acq On : 02 Oct 2024 23:36
 Operator : RC/JU
 Sample : P4010-08DL 5X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AW9DL

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-BP092424.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP022174.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.222	35	40	44	rBV5	3927	5565	0.20%	0.023%
2	3.658	110	114	122	rVB5	4589	10257	0.37%	0.042%
3	3.728	124	126	135	rVB6	4498	7275	0.26%	0.029%
4	3.952	160	164	171	rVB2	7991	11193	0.40%	0.045%
5	4.169	198	201	207	rVB6	5016	7216	0.26%	0.029%
6	4.581	267	271	276	rVB7	2319	3119	0.11%	0.013%
7	4.858	315	318	324	rVB5	2893	4984	0.18%	0.020%
8	4.952	330	334	338	rVB7	2591	3471	0.12%	0.014%
9	5.381	401	407	413	rVB8	2428	5010	0.18%	0.020%
10	6.405	575	581	589	rVB7	5350	9408	0.34%	0.038%
11	6.716	629	634	638	rBV7	3286	5073	0.18%	0.021%
12	6.887	653	663	673	rBV2	49017	105769	3.78%	0.429%
13	7.034	682	688	695	rBV	39752	63016	2.25%	0.255%
14	7.240	716	723	731	rVB	52759	86292	3.09%	0.350%
15	7.693	793	800	808	rBV	424593	700815	25.07%	2.839%
16	7.846	822	826	831	rBV7	2662	4550	0.16%	0.018%
17	8.275	895	899	905	rVB9	1387	3100	0.11%	0.013%
18	8.399	913	920	932	rBV	53152	95330	3.41%	0.386%
19	8.505	932	938	947	rVB	30581	51905	1.86%	0.210%
20	8.781	975	985	988	rBV	2658	5310	0.19%	0.022%
21	8.834	988	994	1002	rVV	45575	79174	2.83%	0.321%
22	8.905	1002	1006	1010	rVB6	4427	6037	0.22%	0.024%
23	9.257	1062	1066	1071	rBV7	2560	3645	0.13%	0.015%
24	9.552	1109	1116	1122	rBV3	34221	64315	2.30%	0.261%
25	9.663	1130	1135	1138	rBV7	1452	2956	0.11%	0.012%
26	9.710	1138	1143	1153	rVV2	16701	39995	1.43%	0.162%
27	9.781	1153	1155	1166	rVV9	5960	12669	0.45%	0.051%
28	9.904	1169	1176	1183	rBV10	4413	11966	0.43%	0.048%
29	10.087	1200	1207	1215	rBV	60129	110471	3.95%	0.448%
30	10.457	1261	1270	1279	rBV	574223	1019528	36.47%	4.131%
31	10.551	1279	1286	1291	rVV2	18713	38044	1.36%	0.154%
32	10.599	1291	1294	1301	rVB5	8913	17572	0.63%	0.071%
33	10.875	1336	1341	1348	rVB2	6938	12765	0.46%	0.052%
34	10.993	1356	1361	1365	rBV8	5652	8766	0.31%	0.036%
35	11.251	1396	1405	1411	rBV8	5422	12703	0.45%	0.051%
36	11.816	1494	1501	1505	rVB10	1983	3293	0.12%	0.013%

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37	12.228	1565	1571	1578	rBV	14236	34977	1.25%	0.142%
38	12.575	1623	1630	1633	rBV8	2800	5560	0.20%	0.023%
39	12.657	1639	1644	1649	rBV8	4355	7424	0.27%	0.030%
40	12.851	1671	1677	1683	rVB10	1506	3143	0.11%	0.013%
41	13.181	1728	1733	1737	rBV8	6153	9848	0.35%	0.040%
42	13.304	1748	1754	1758	rVB9	1591	3071	0.11%	0.012%
43	13.416	1768	1773	1777	rBV8	3768	8296	0.30%	0.034%
44	13.622	1797	1808	1817	rBV4	21286	45791	1.64%	0.186%
45	13.710	1817	1823	1833	rVV	139348	197630	7.07%	0.801%
46	13.787	1834	1836	1841	rVB6	1833	3185	0.11%	0.013%
47	13.845	1841	1846	1849	rBV7	1751	3604	0.13%	0.015%
48	13.892	1849	1854	1859	rBV8	3346	5809	0.21%	0.024%
49	13.992	1865	1871	1882	rVB	139713	203221	7.27%	0.823%
50	14.151	1890	1898	1907	rBV4	20469	51150	1.83%	0.207%
51	14.310	1915	1925	1933	rBV	1171282	1582146	56.59%	6.410%
52	14.375	1934	1936	1944	rVB6	9247	14594	0.52%	0.059%
53	14.545	1957	1965	1975	rBV8	18334	64053	2.29%	0.260%
54	14.628	1977	1979	1985	rVB4	4352	7662	0.27%	0.031%
55	14.734	1992	1997	2002	rVB3	15044	22208	0.79%	0.090%
56	14.887	2021	2023	2027	rBV5	1786	2803	0.10%	0.011%
57	15.316	2090	2096	2107	rVB	209565	296239	10.60%	1.200%
58	15.434	2111	2116	2123	rBV	32342	45958	1.64%	0.186%
59	15.563	2135	2138	2143	rVB7	3135	4880	0.17%	0.020%
60	15.687	2152	2159	2167	rBV	35939	63921	2.29%	0.259%
61	15.810	2177	2180	2185	rVB7	6283	9982	0.36%	0.040%
62	15.916	2189	2198	2202	rBV7	6325	16278	0.58%	0.066%
63	15.975	2204	2208	2211	rBV6	3803	7416	0.27%	0.030%
64	16.057	2218	2222	2226	rBV6	4015	6327	0.23%	0.026%
65	16.192	2240	2245	2248	rBV7	8497	12960	0.46%	0.053%
66	16.504	2293	2298	2304	rBV4	17582	28107	1.01%	0.114%
67	16.675	2325	2327	2331	rBV5	2760	3150	0.11%	0.013%
68	16.751	2336	2340	2348	rVB7	21493	31446	1.12%	0.127%
69	16.869	2358	2360	2364	rBV5	5104	6092	0.22%	0.025%
70	16.992	2376	2381	2382	rBV5	6934	10728	0.38%	0.043%
71	17.016	2382	2385	2389	rVV2	25729	36007	1.29%	0.146%
72	17.104	2393	2400	2408	rVV	1521826	2004542	71.70%	8.122%
73	17.204	2411	2417	2427	rVB	176244	286702	10.26%	1.162%
74	17.345	2438	2441	2446	rBV6	10368	16869	0.60%	0.068%
75	17.410	2449	2452	2459	rVB	10027	16089	0.58%	0.065%
76	17.639	2487	2491	2495	rBV5	11730	15095	0.54%	0.061%

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77	18.045	2556	2560	2566	rBV	148743	195309	6.99%	0.791%
78	18.116	2569	2572	2576	rVB	29557	39320	1.41%	0.159%
79	18.357	2611	2613	2618	rBV3	24624	27371	0.98%	0.111%
80	19.022	2723	2726	2730	rBV2	27854	37233	1.33%	0.151%
81	19.375	2783	2786	2790	rBV4	44638	64809	2.32%	0.263%
82	19.586	2817	2822	2826	rBV	267748	354994	12.70%	1.438%
83	20.574	2985	2990	2995	rBV	1804779	2215848	79.26%	8.978%
84	21.010	3060	3064	3070	rBV	219212	302672	10.83%	1.226%
85	21.204	3093	3097	3110	rVB2	281041	621601	22.23%	2.518%
86	21.427	3131	3135	3136	rBV	183679	204783	7.33%	0.830%
87	21.533	3148	3153	3159	rBV2	1405639	2174350	77.78%	8.809%
88	22.427	3299	3305	3318	rVB2	567811	1542388	55.17%	6.249%
89	23.968	3560	3567	3574	rBV	1287807	2795652	100.00%	11.327%
90	24.821	3703	3712	3725	rBV2	847514	2468507	88.30%	10.001%
91	26.121	3925	3933	3944	rVB	882700	2526108	90.36%	10.235%
92	28.009	4247	4254	4272	rVB2	355792	1283440	45.91%	5.200%

Sum of corrected areas: 24681905

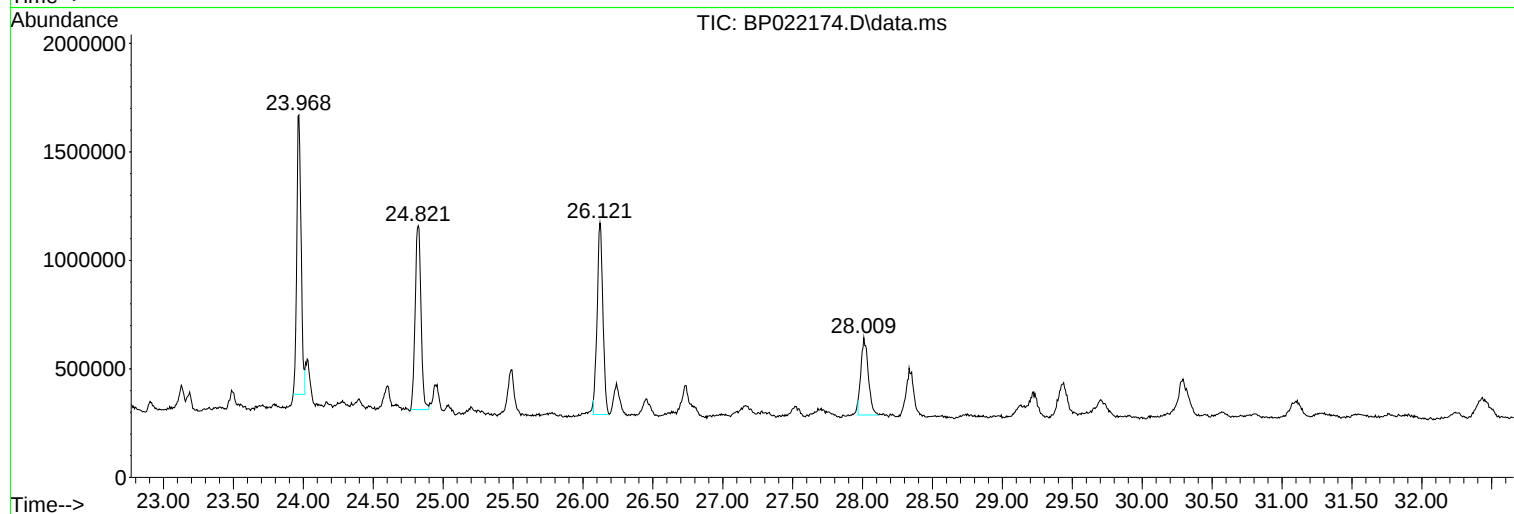
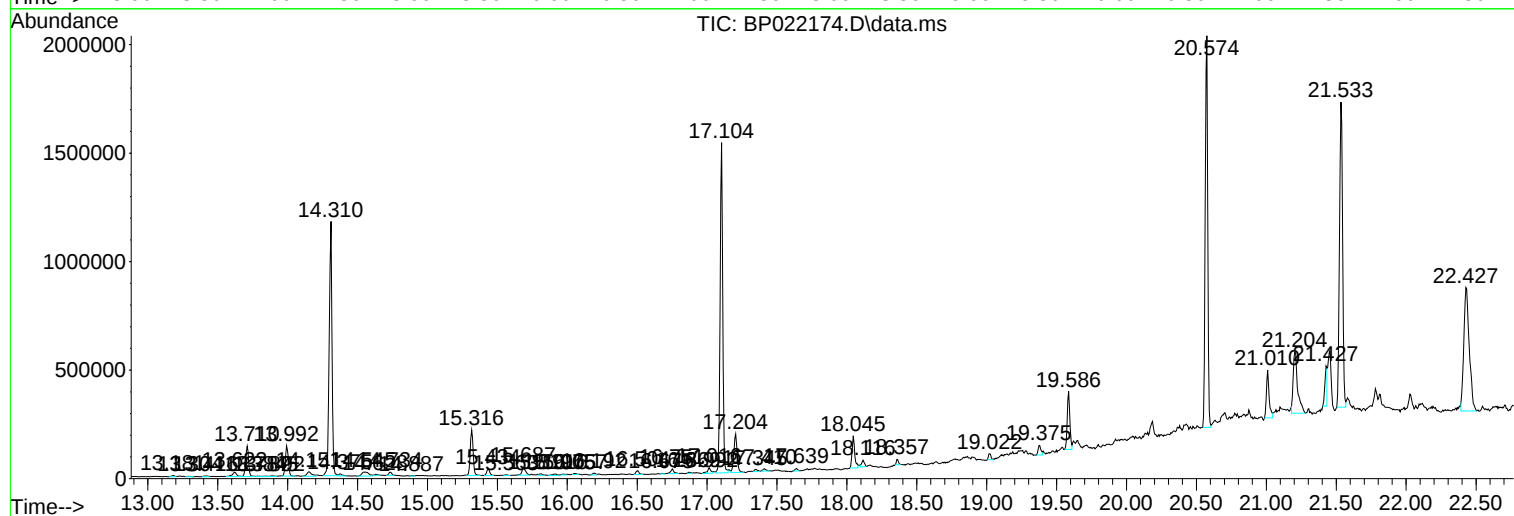
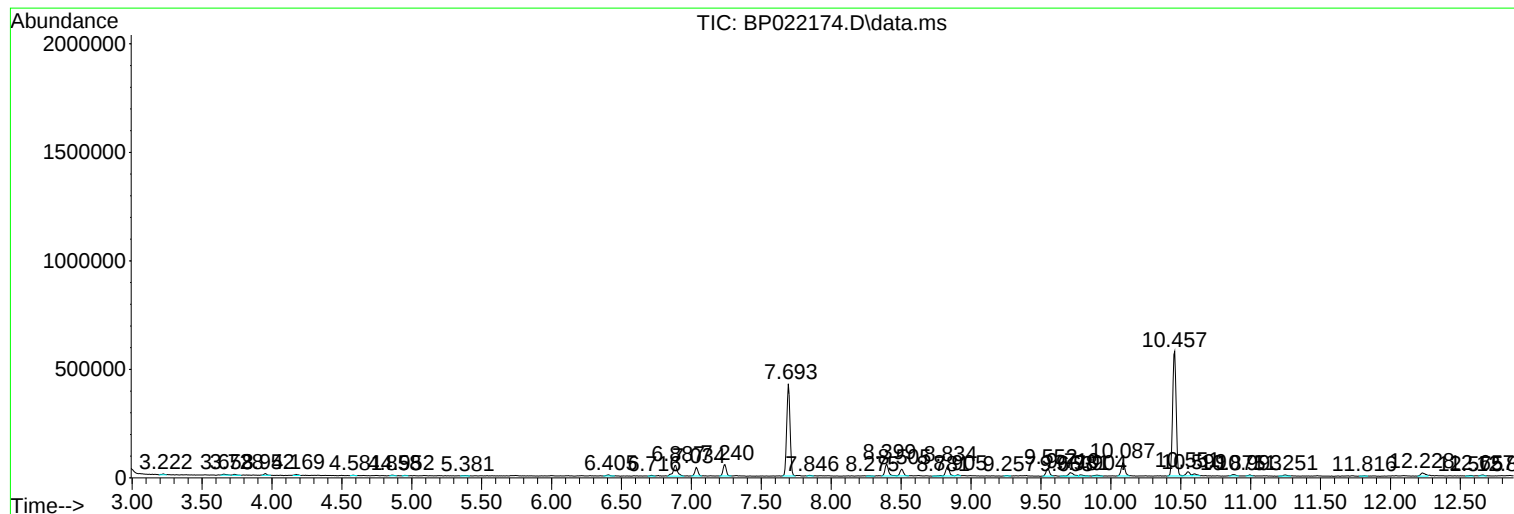
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST20.L

TIC Integration Parameters: LSCINT.P



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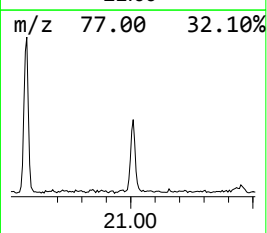
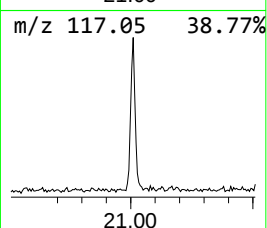
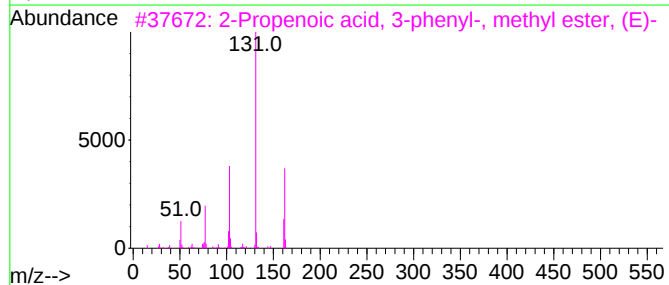
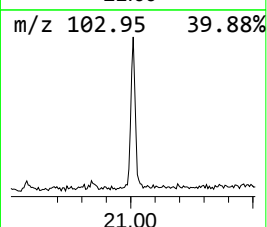
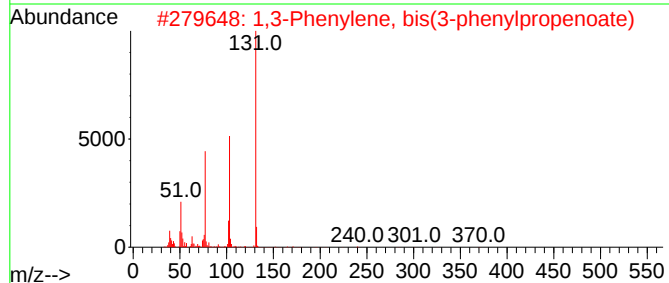
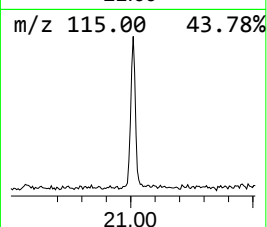
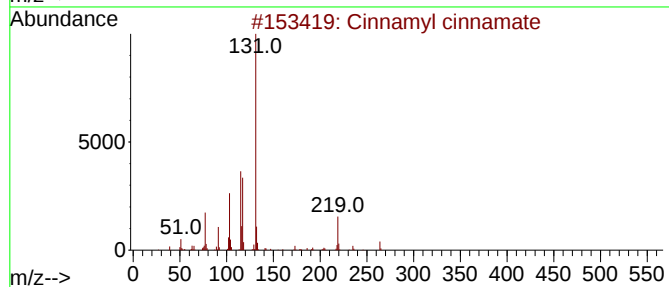
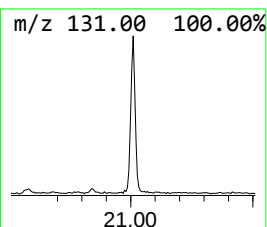
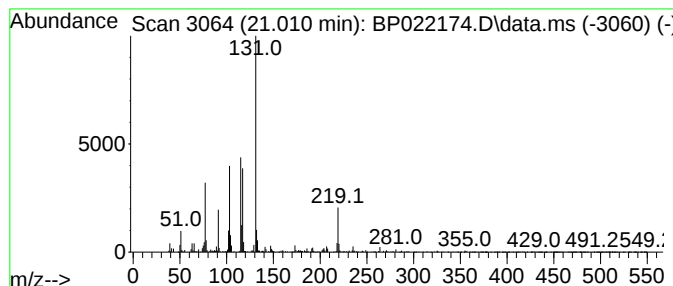
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Cinnamyl cinnamate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	2.78 ng/ul	302672	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2			1,3-Phenylene, bis(3-phenylprope...	370	C24H18O4	1000259-62-4	55
3			2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	47
4			N-(2-Methyl-1,3-dioxo-5-isoindol...	306	C18H14N2O3	1000224-44-2	46
5			Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	46



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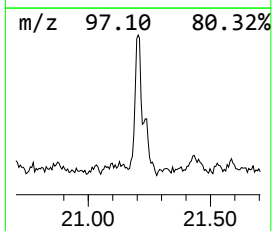
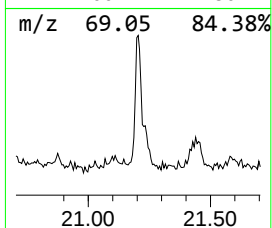
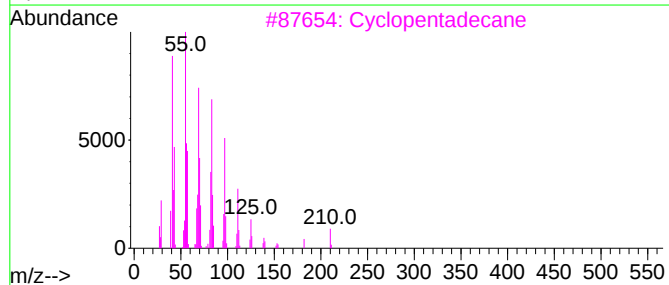
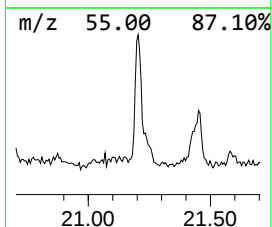
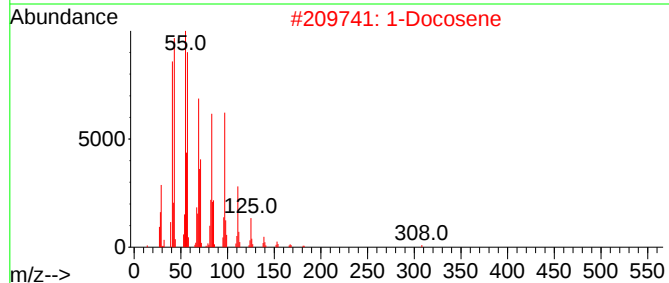
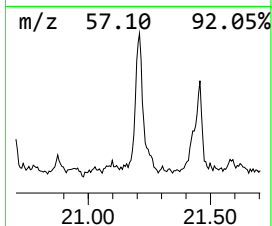
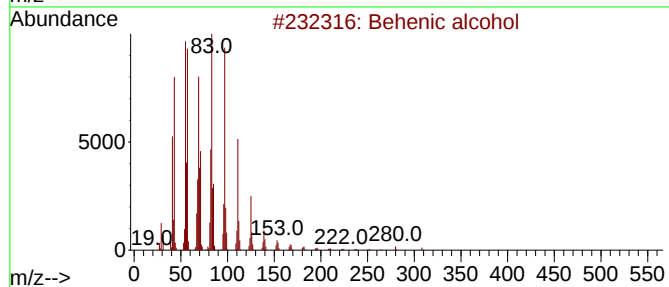
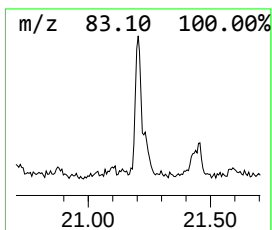
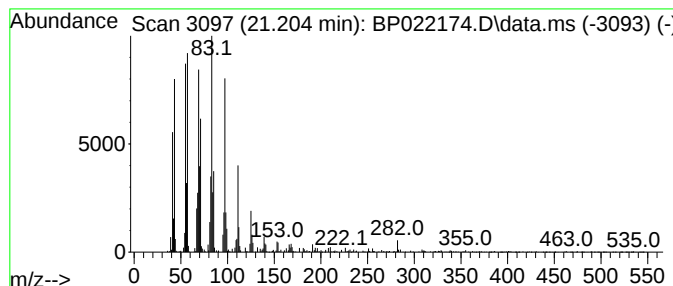
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	5.72 ng/ul	621601	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			1-Docosene	308	C22H44	001599-67-3	94
3			Cyclopentadecane	210	C15H30	000295-48-7	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5			Nonacos-1-ene	406	C29H58	018835-35-3	93



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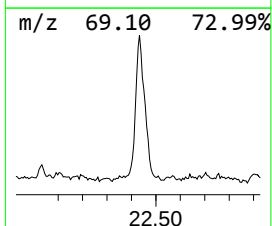
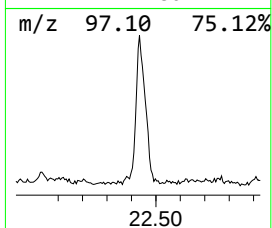
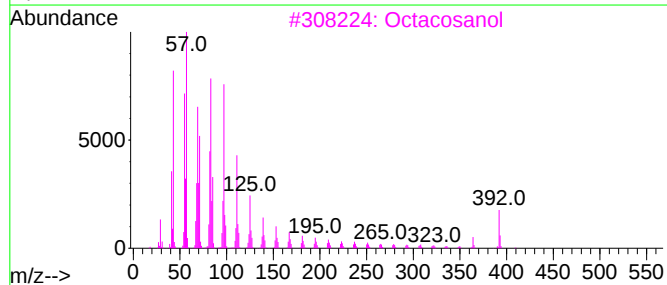
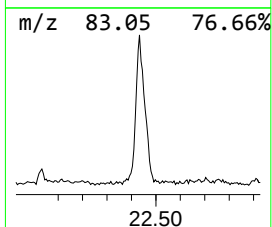
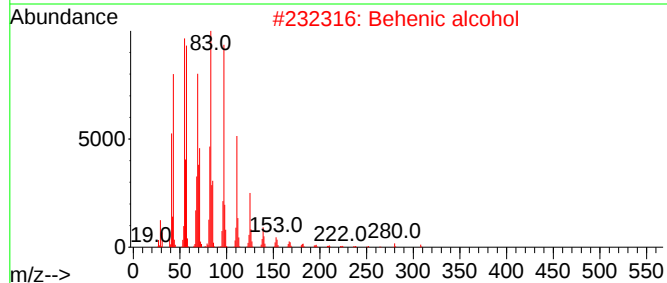
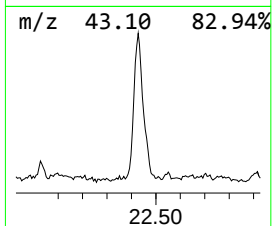
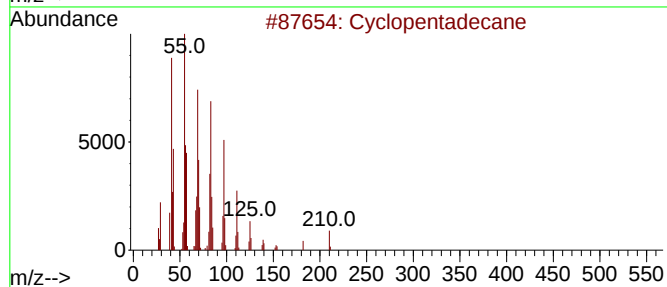
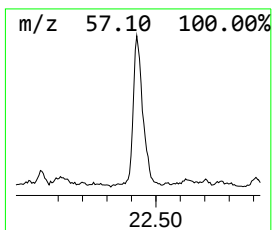
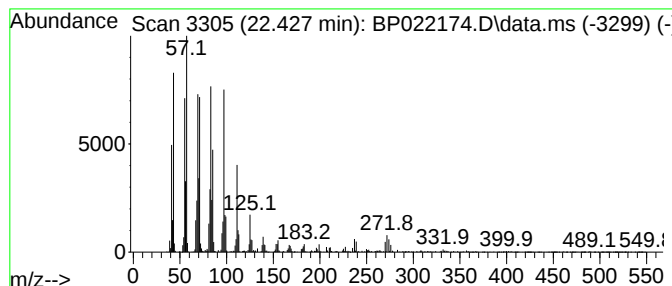
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 (DEL) Alkane: Cyclic22.427 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.427	14.19 ng/ul	1542390	Chrysene-d12	21.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	95
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			Octacosanol	410	C28H58O	000557-61-9	91
4			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5			1-Tetracosene	336	C24H48	010192-32-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022174.D
Acq On : 02 Oct 2024 23:36
Operator : RC/JU
Sample : P4010-08DL 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

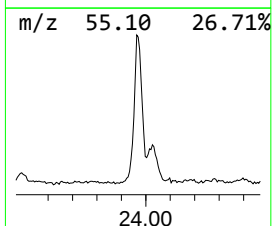
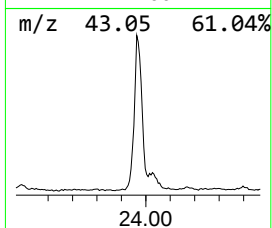
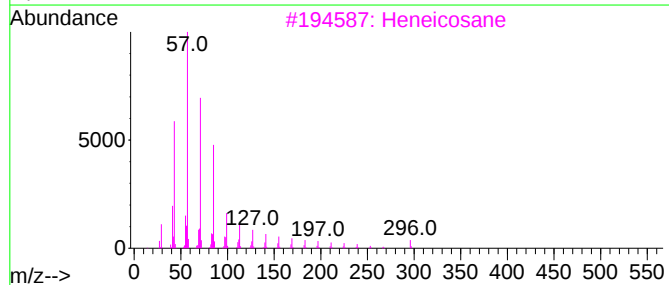
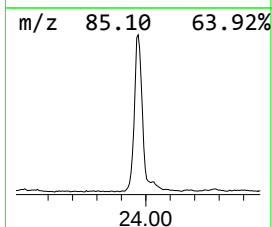
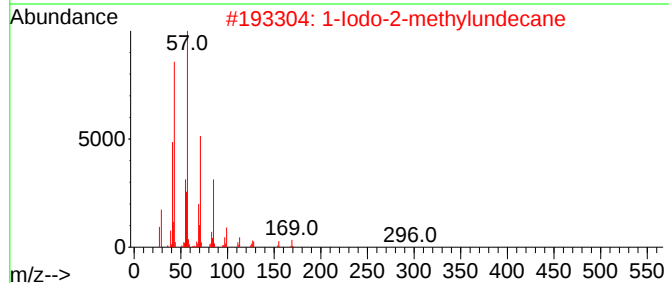
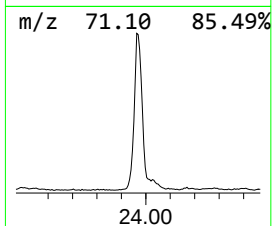
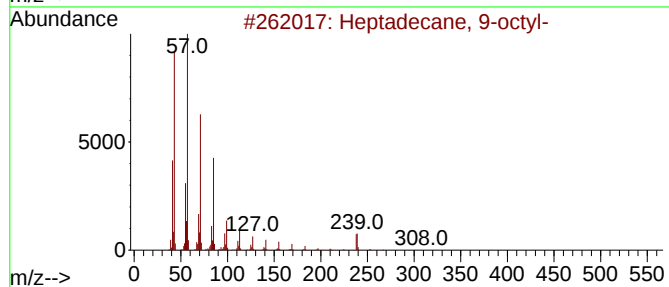
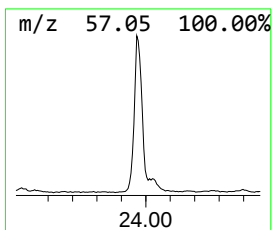
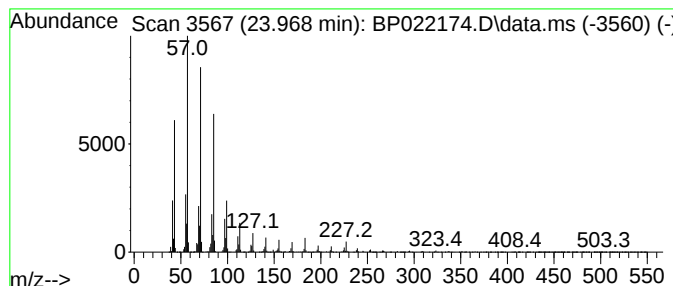
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.968	22.65 ng/ul	2795650	Perylene-d12	24.821	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Pentacosane	352	C25H52	000629-99-2	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022174.D
Acq On : 02 Oct 2024 23:36
Operator : RC/JU
Sample : P4010-08DL 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AW9DL

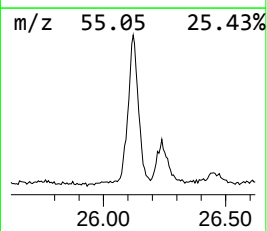
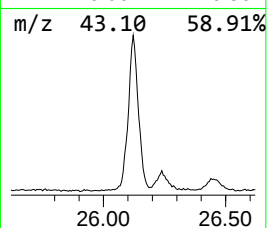
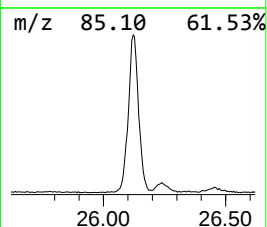
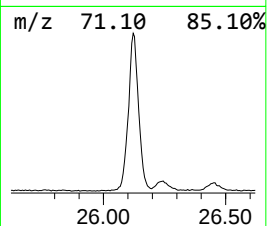
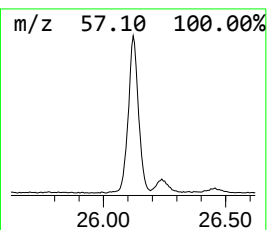
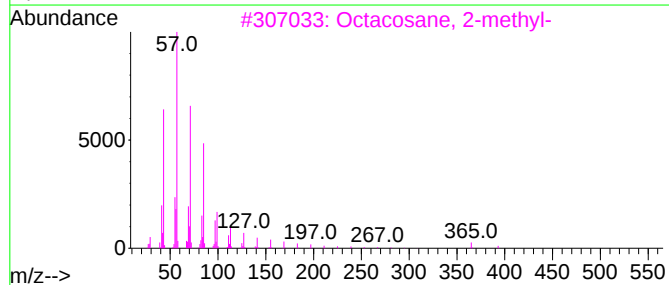
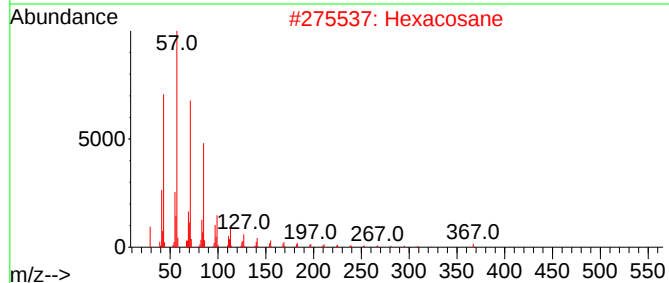
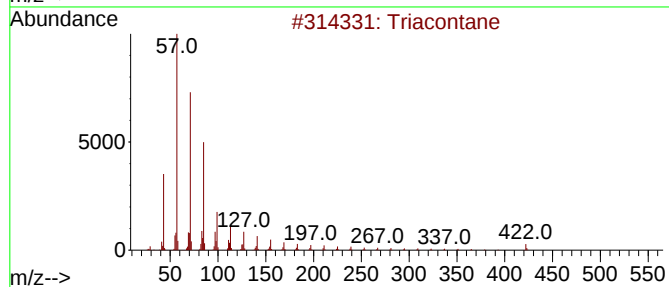
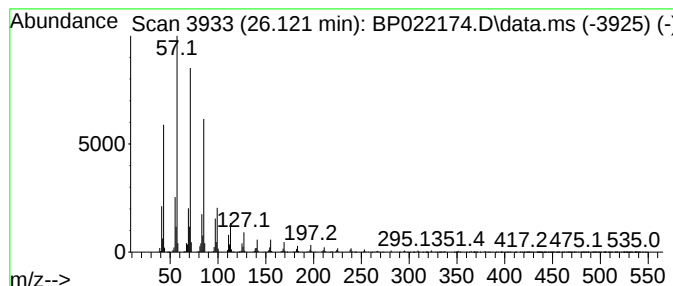
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.121	20.47 ng/ul	2526110	Perylene-d12	24.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane, 9-octyl-	479	C34H70	055429-83-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022174.D
Acq On : 02 Oct 2024 23:36
Operator : RC/JU
Sample : P4010-08DL 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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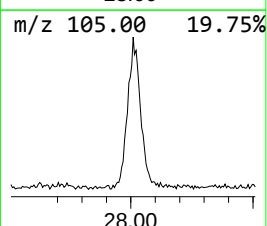
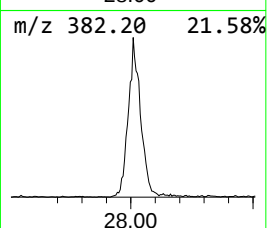
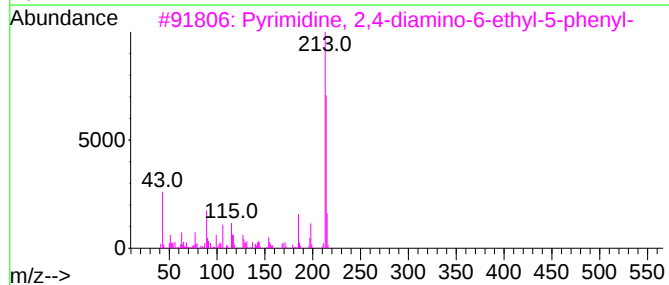
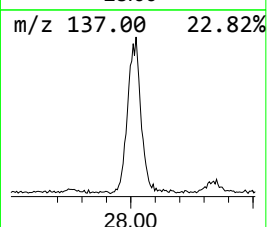
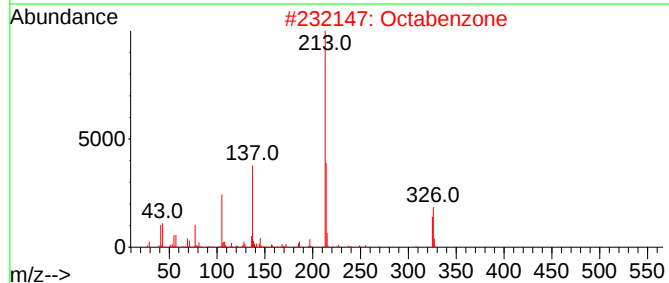
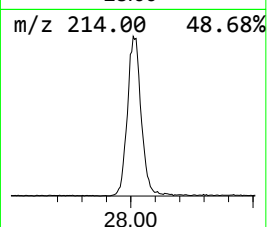
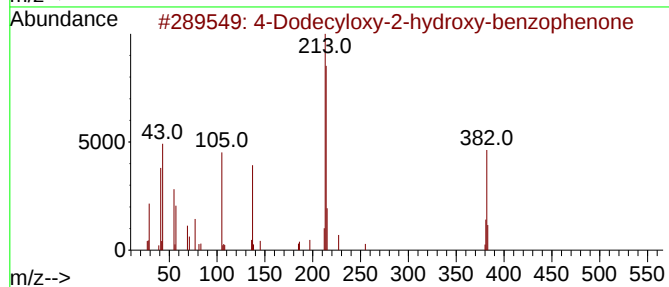
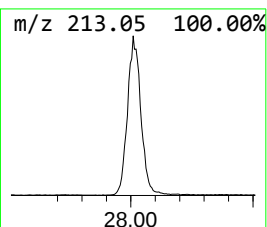
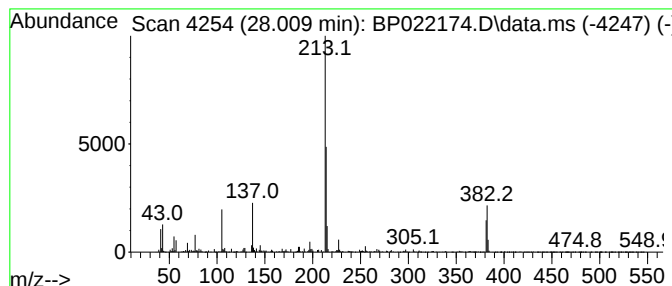
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 4-Dodecyloxy-2-hydroxy-benz... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.009	10.40 ng/ul	1283440	Perylene-d12	24.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Dodecyloxy-2-hydroxy-benzophenone	382	C25H34O3	1000425-91-3	96
2			Octabenzene	326	C21H26O3	001843-05-6	43
3			Pyrimidine, 2,4-diamino-6-ethyl-...	214	C12H14N4	027653-49-2	38
4			Thiazolo[4,5-d]pyrimidin-7(4H)-o...	213	C7H7N3OS2	119011-51-7	35
5			Propenenitrile, 3-(4-morpholyl)-...	214	C13H14N2O	020842-95-9	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100224\
Data File : BP022174.D
Acq On : 02 Oct 2024 23:36
Operator : RC/JU
Sample : P4010-08DL 5X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AW9DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP092424.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
Cinnamyl cinnamate	21.010	2.8	ng/ul	302672	5	21.533	2174350	20.0
Behenic alcohol	21.204	5.7	ng/ul	621601	5	21.533	2174350	20.0
(DEL) Alkane: C...	22.427	14.2	ng/ul	1542390	5	21.533	2174350	20.0
(DEL) Alkane: S...	23.968	22.6	ng/ul	2795650	6	24.821	2468510	20.0
(DEL) Alkane: S...	26.121	20.5	ng/ul	2526110	6	24.821	2468510	20.0
4-Dodecyloxy-2-...	28.009	10.4	ng/ul	1283440	6	24.821	2468510	20.0