

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070824\
 Data File : BP020863.D
 Acq On : 09 Jul 2024 14:01
 Operator : MA/JU
 Sample : P3084-07
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 E1G89

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-BP062524.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP020863.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.264	43	47	56	rVB	41967	61775	1.29%	0.109%
2	3.540	91	94	100	rBV	35996	53305	1.11%	0.094%
3	3.699	119	121	127	rBV	17249	29881	0.62%	0.053%
4	3.987	166	170	175	rVB	14849	19636	0.41%	0.035%
5	4.405	237	241	245	rVB3	6560	8730	0.18%	0.015%
6	4.770	299	303	307	rBV6	5185	7108	0.15%	0.013%
7	4.881	317	322	326	rBV	12495	20392	0.42%	0.036%
8	5.711	459	463	467	rVV6	3381	5319	0.11%	0.009%
9	5.775	467	474	477	rVB9	4491	7431	0.15%	0.013%
10	5.846	482	486	493	rVV	22463	35786	0.74%	0.063%
11	6.011	512	514	519	rBV6	4372	6768	0.14%	0.012%
12	6.381	571	577	582	rVB10	5291	10598	0.22%	0.019%
13	6.781	640	645	650	rBV7	4437	8027	0.17%	0.014%
14	6.922	663	669	681	rVB	244388	439112	9.14%	0.776%
15	7.069	687	694	706	rBV	665871	1013208	21.08%	1.791%
16	7.269	722	728	737	rBV	780998	1272891	26.49%	2.250%
17	7.346	738	741	750	rVV4	16467	42037	0.87%	0.074%
18	7.422	750	754	758	rVB7	7737	11532	0.24%	0.020%
19	7.722	795	805	812	rBV	692328	1159279	24.12%	2.049%
20	7.793	812	817	831	rVB2	30212	76716	1.60%	0.136%
21	8.269	894	898	904	rVB7	3649	6756	0.14%	0.012%
22	8.334	904	909	910	rBV5	5070	5957	0.12%	0.011%
23	8.434	919	926	940	rBV	657033	1167209	24.29%	2.063%
24	8.881	994	1002	1014	rBV	759115	1327472	27.62%	2.347%
25	9.022	1020	1026	1032	rVB9	9469	20428	0.43%	0.036%
26	9.240	1058	1063	1070	rVB2	23116	40632	0.85%	0.072%
27	9.428	1089	1095	1108	rVB	76556	132065	2.75%	0.233%
28	9.587	1115	1122	1134	rBV	651250	1141533	23.75%	2.018%
29	9.811	1153	1160	1161	rBV7	3229	5640	0.12%	0.010%
30	9.840	1163	1165	1170	rVB6	5231	7765	0.16%	0.014%
31	10.134	1206	1215	1231	rBV	973151	1723405	35.86%	3.047%
32	10.499	1266	1277	1289	rBV	1040156	1692751	35.22%	2.992%
33	10.640	1294	1301	1315	rVV	449124	895263	18.63%	1.583%
34	10.734	1315	1317	1324	rVB8	6079	9836	0.20%	0.017%
35	11.034	1361	1368	1376	rBV8	14817	36235	0.75%	0.064%
36	11.169	1384	1391	1396	rVB10	3015	7082	0.15%	0.013%

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ClientSampleId :
E1G89

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_P\Methods\SFAM-EPA-BP062524.MA.M
Title : SVOA CALIBRATION

37	11.240	1396	1403	1412	rBV	97223	222450	4.63%	0.393%
38	11.905	1511	1516	1521	rVB4	10684	15927	0.33%	0.028%
39	12.081	1540	1546	1555	rVB3	12429	26587	0.55%	0.047%
40	12.163	1555	1560	1561	rBV5	6481	6550	0.14%	0.012%
41	12.322	1585	1587	1595	rVB8	2875	5599	0.12%	0.010%
42	12.716	1653	1654	1659	rVB5	5379	6363	0.13%	0.011%
43	12.810	1666	1670	1675	rVV8	3167	6644	0.14%	0.012%
44	12.869	1675	1680	1688	rVB8	5195	11624	0.24%	0.021%
45	13.157	1720	1729	1734	rBV2	21210	34652	0.72%	0.061%
46	13.316	1752	1756	1762	rVB7	6680	10502	0.22%	0.019%
47	13.534	1788	1793	1797	rBV	6046	9064	0.19%	0.016%
48	13.769	1824	1833	1846	rBV	1921613	2509667	52.22%	4.437%
49	13.869	1849	1850	1857	rVB7	6013	6459	0.13%	0.011%
50	14.057	1869	1882	1888	rBV	2028552	3065449	63.79%	5.419%
51	14.246	1906	1914	1917	rBV6	12666	16645	0.35%	0.029%
52	14.363	1923	1934	1940	rBV	1658763	2346084	48.82%	4.147%
53	14.581	1964	1971	1974	rBV	72135	156933	3.27%	0.277%
54	14.616	1974	1977	1989	rVB	136084	266326	5.54%	0.471%
55	14.751	1997	2000	2004	rBV6	3315	6614	0.14%	0.012%
56	14.793	2004	2007	2020	rVV6	13492	33915	0.71%	0.060%
57	14.893	2020	2024	2028	rVB7	6122	11103	0.23%	0.020%
58	14.951	2031	2034	2037	rVB5	4583	5736	0.12%	0.010%
59	15.163	2066	2070	2075	rBV3	17769	28749	0.60%	0.051%
60	15.222	2075	2080	2083	rVV3	14703	21539	0.45%	0.038%
61	15.369	2098	2105	2113	rBV	2512238	3723345	77.48%	6.582%
62	15.428	2113	2115	2125	rVB9	19398	29586	0.62%	0.052%
63	15.522	2125	2131	2141	rBV	312057	606489	12.62%	1.072%
64	15.616	2144	2147	2154	rVB6	15461	26679	0.56%	0.047%
65	15.746	2166	2169	2174	rVB6	7851	12522	0.26%	0.022%
66	15.804	2174	2179	2183	rVB7	10094	15917	0.33%	0.028%
67	15.957	2201	2205	2210	rBV7	10254	19622	0.41%	0.035%
68	16.057	2218	2222	2224	rBV4	5581	8715	0.18%	0.015%
69	16.098	2226	2229	2236	rVB4	18515	32427	0.67%	0.057%
70	16.263	2254	2257	2258	rBV3	5931	6384	0.13%	0.011%
71	16.434	2283	2286	2289	rBV5	10025	13295	0.28%	0.024%
72	16.569	2304	2309	2315	rBV5	40205	80462	1.67%	0.142%
73	16.675	2324	2327	2329	rBV2	17566	24878	0.52%	0.044%
74	16.704	2329	2332	2336	rVB5	22968	35640	0.74%	0.063%
75	16.922	2366	2369	2373	rBV3	14442	20499	0.43%	0.036%
76	17.098	2395	2399	2402	rBV2	32575	38116	0.79%	0.067%

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 Sampling : 1 Min Area: 0.1 % of largest Peak
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 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

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77	17.175	2403	2412	2418	rBV	1989985	2824264	58.77%	4.993%
78	17.275	2423	2429	2438	rVV2	2499740	4169115	86.76%	7.370%
79	17.363	2440	2444	2449	rVB3	26568	41092	0.86%	0.073%
80	17.481	2458	2464	2472	rBV8	36390	103503	2.15%	0.183%
81	17.875	2528	2531	2537	rVB	31912	42396	0.88%	0.075%
82	17.969	2543	2547	2557	rVB3	77397	121413	2.53%	0.215%
83	18.122	2567	2573	2583	rBV	796356	1255218	26.12%	2.219%
84	19.445	2794	2798	2805	rBV3	159246	287574	5.98%	0.508%
85	19.663	2829	2835	2841	rBV2	3224009	4805575	100.00%	8.495%
86	19.781	2852	2855	2856	rBV3	101543	106036	2.21%	0.187%
87	19.828	2858	2863	2867	rVB8	114171	226958	4.72%	0.401%
88	19.898	2873	2875	2876	rBV2	49330	36348	0.76%	0.064%
89	20.216	2927	2929	2930	rBV	92938	68841	1.43%	0.122%
90	20.233	2930	2932	2935	rVV3	92856	92771	1.93%	0.164%
91	20.563	2984	2988	2990	rBV3	333428	359407	7.48%	0.635%
92	21.298	3108	3113	3117	rBV	977893	1546588	32.18%	2.734%
93	21.351	3120	3122	3126	rVB4	172542	246362	5.13%	0.436%
94	21.633	3164	3170	3176	rBV2	1690631	2932497	61.02%	5.184%
95	22.063	3239	3243	3245	rBV4	242730	376770	7.84%	0.666%
96	22.092	3245	3248	3259	rVB7	358179	792191	16.48%	1.400%
97	23.422	3468	3474	3481	rBV	881070	1849090	38.48%	3.269%
98	23.492	3484	3486	3488	rBV2	175314	140010	2.91%	0.248%
99	24.751	3692	3700	3711	rVB2	1756773	4751860	98.88%	8.400%
100	24.980	3732	3739	3751	rVB	1205709	3356893	69.85%	5.934%

Sum of corrected areas: 56568089

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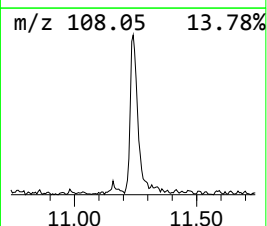
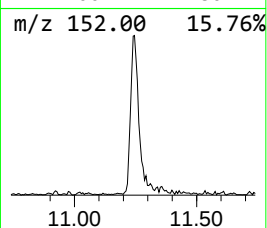
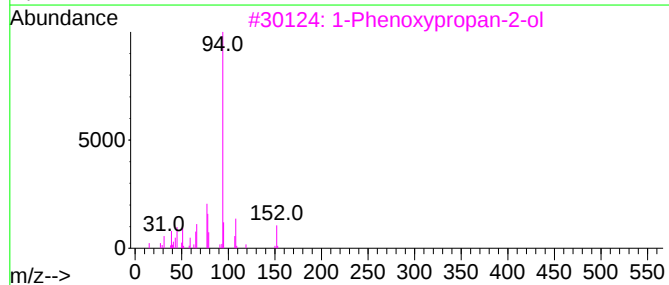
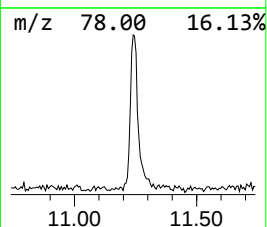
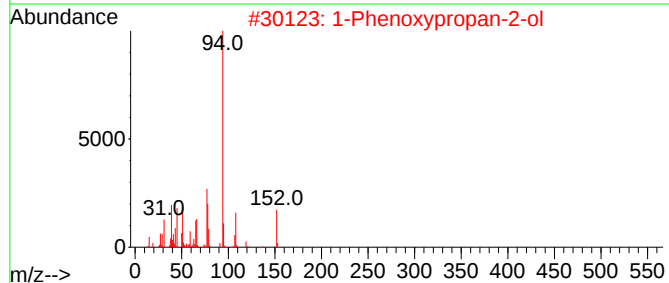
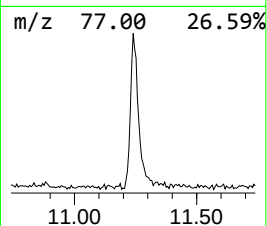
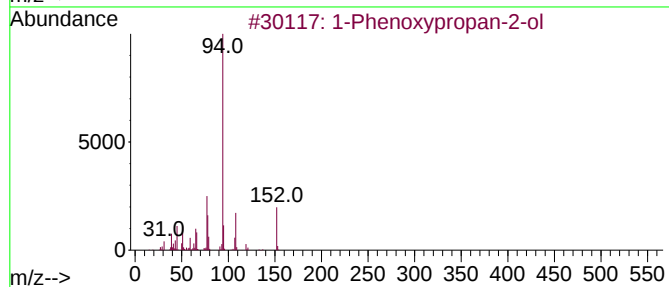
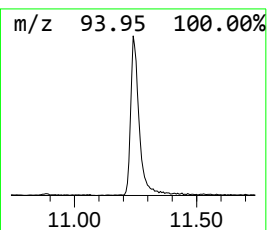
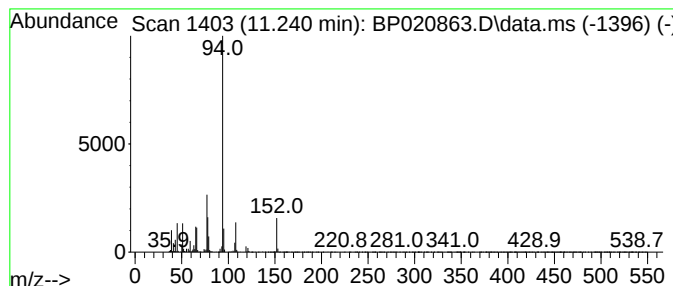
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.240	2.63 ng/ul	222450	Naphthalene-d8	10.499

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
4			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
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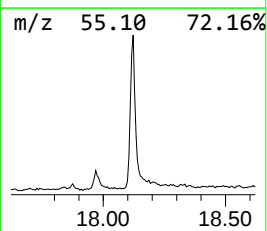
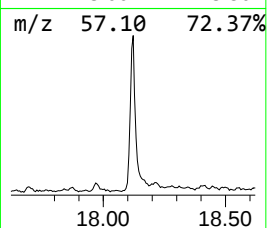
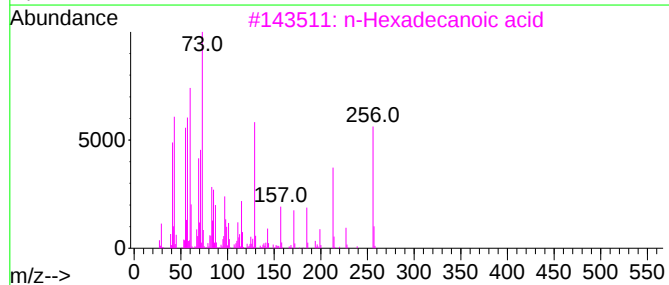
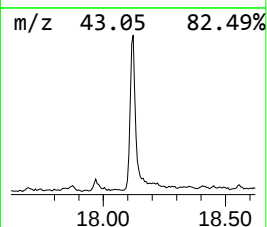
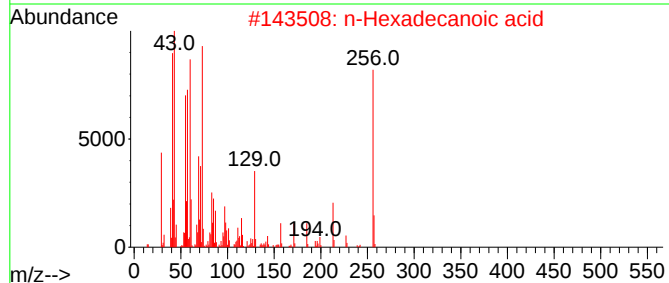
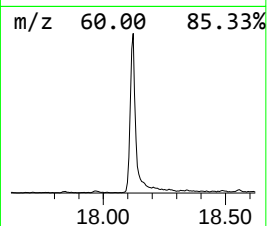
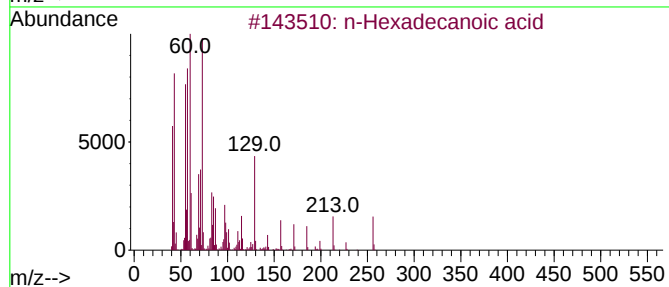
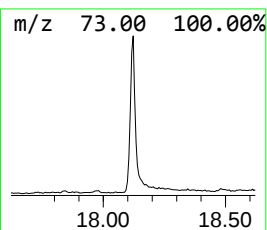
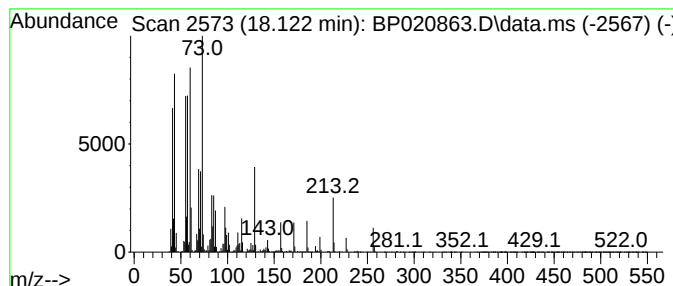
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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.
18.122	8.89 ng/ul	1255220	Phenanthrene-d10	17.175

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	98
5			Tridecanoic acid	214	C13H26O2	000638-53-9	95



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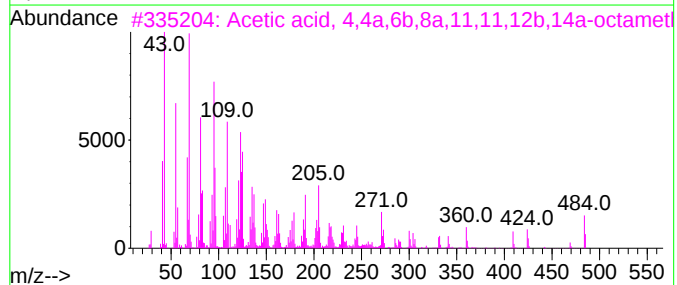
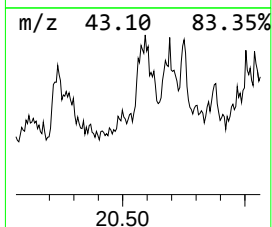
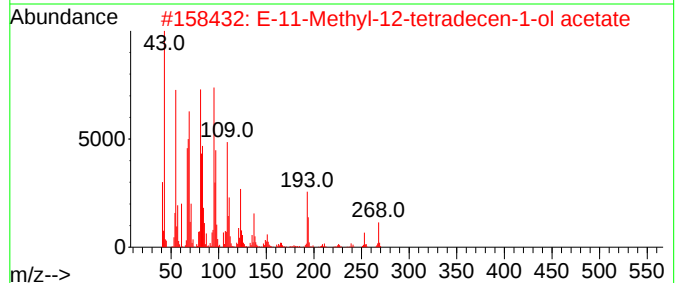
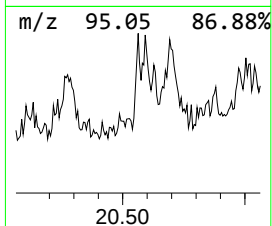
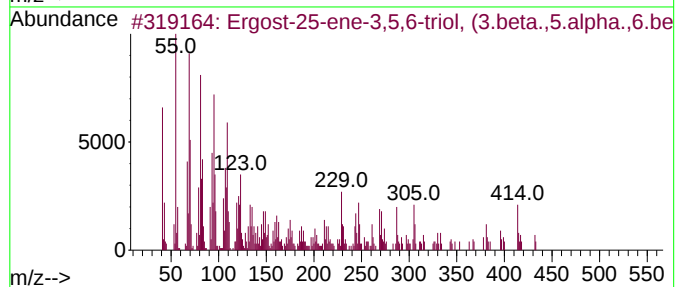
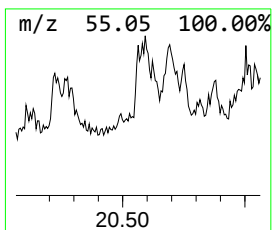
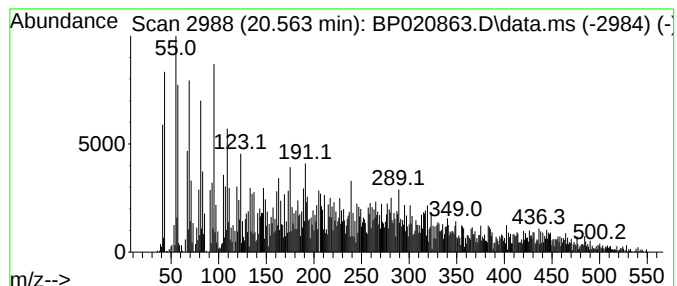
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Ergost-25-ene-3,5,6-triol, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.563	2.45 ng/ul	359407	Chrysene-d12	21.633	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ergost-25-ene-3,5,6-triol, (3.be...	432	C28H48O3	056143-28-3	56
2	E-11-Methyl-12-tetradecen-1-ol a...	268	C17H32O2	1000130-80-7	56
3	Acetic acid, 4,4a,6b,8a,11,11,12...	484	C32H52O3	1000192-72-4	56
4	Lanost-7-en-3-one, (9.beta.,13.a...	426	C30H50O	055515-18-9	55
5	Cyclotriaconta-1,7,16,22-tetraone	476	C30H52O4	1000155-91-6	55



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E1G89

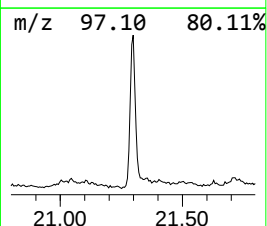
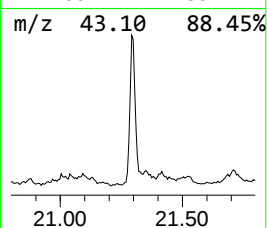
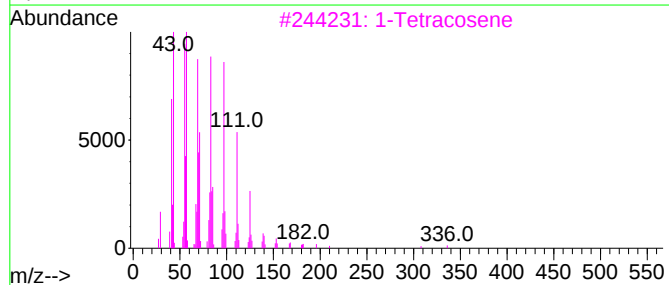
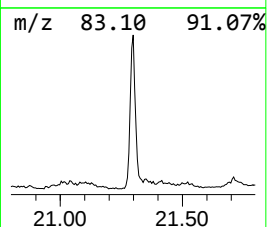
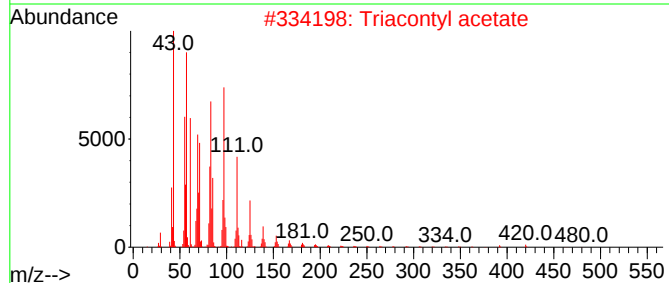
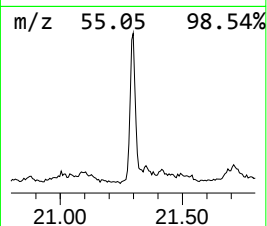
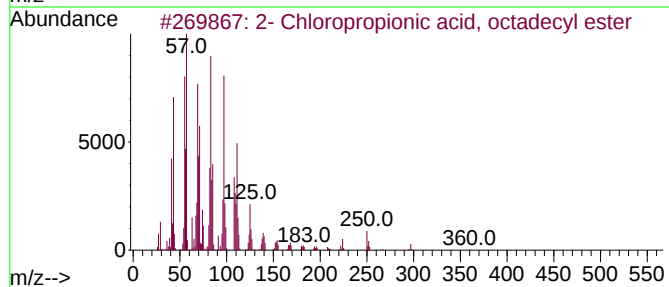
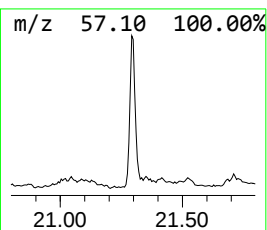
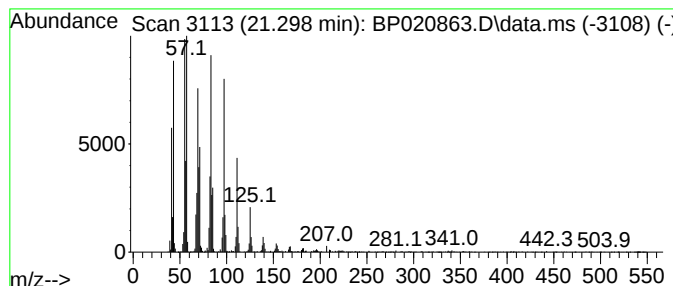
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 2- Chloropropionic acid, oc... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.298	10.55 ng/ul	1546590	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-	Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	97	
2	Triacontyl acetate	480	C32H64O2	041755-58-2	96		
3	1-Tetracosene	336	C24H48	010192-32-2	94		
4	1-Hexacosene	364	C26H52	018835-33-1	94		
5	1-Heneicosanol	312	C21H44O	015594-90-8	94		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070824\
Data File : BP020863.D
Acq On : 09 Jul 2024 14:01
Operator : MA/JU
Sample : P3084-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

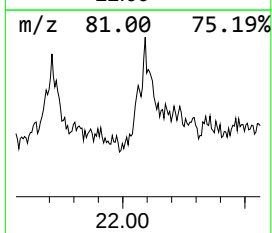
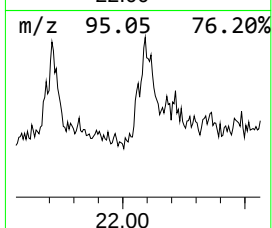
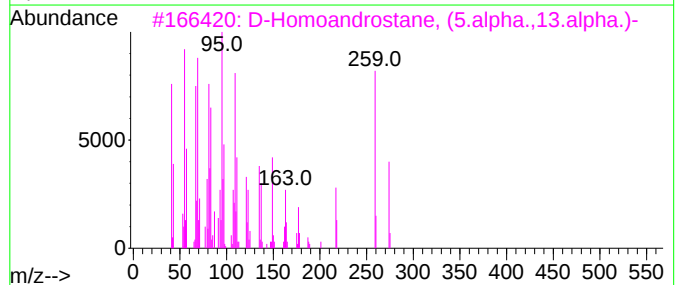
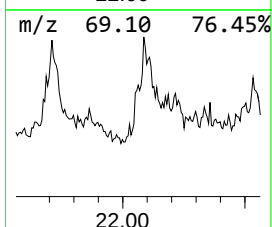
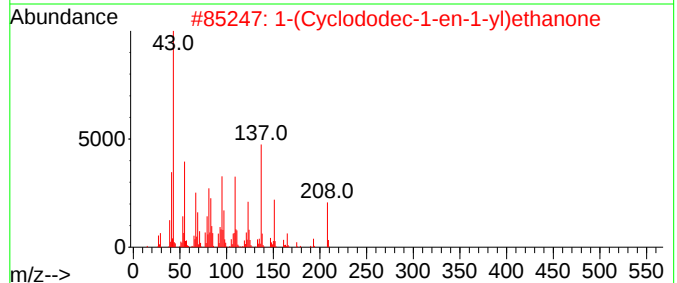
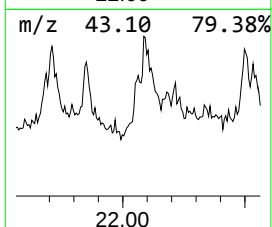
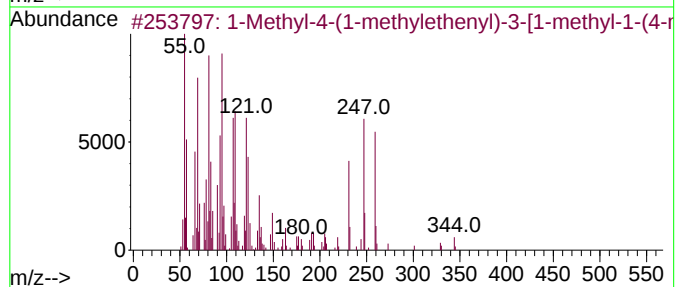
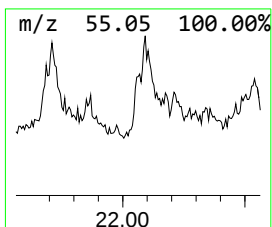
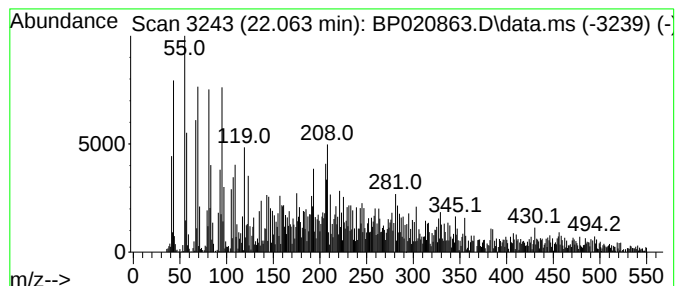
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BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Methyl-4-(1-methylethenyl)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.063	2.57 ng/ul	376770	Chrysene-d12	21.633	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-4-(1-methylethenyl)-3-[...]	344	C25H44	1000370-41-3	86
2	1-(Cyclododec-1-en-1-yl)ethanone	208	C14H24O	065938-08-1	53
3	D-Homoandrostane, (5.alpha.,13.alpha.)	274	C20H34	054482-31-4	51
4	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	49
5	Dichlorophen, 0,0'-di(2-furoyl)-	456	C23H14Cl2O6	1010355-17-8	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070824\
Data File : BP020863.D
Acq On : 09 Jul 2024 14:01
Operator : MA/JU
Sample : P3084-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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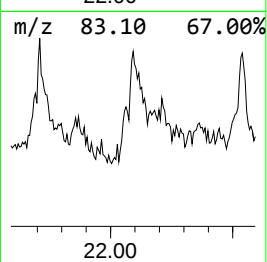
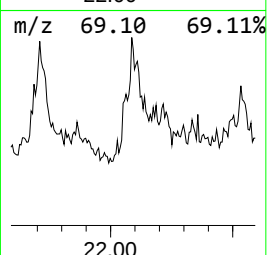
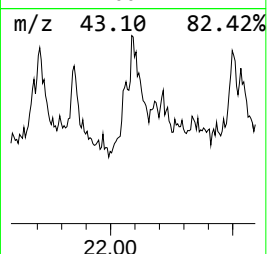
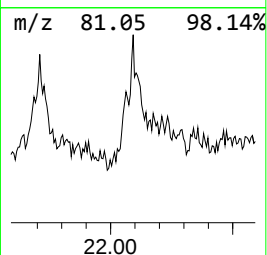
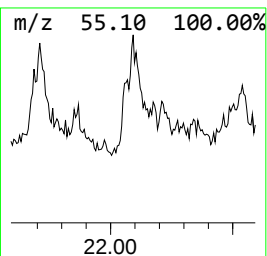
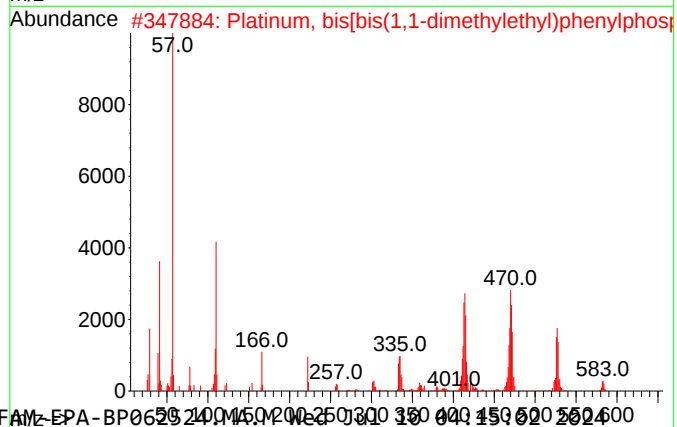
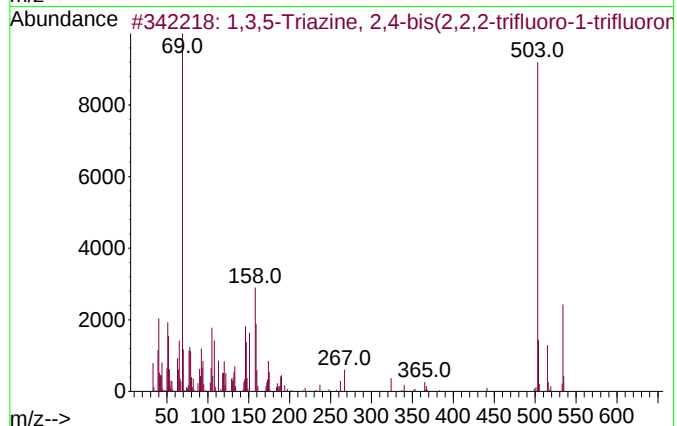
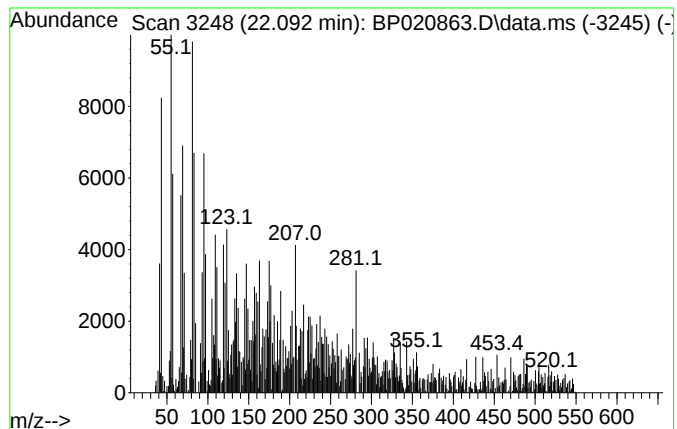
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.092	5.40 ng/ul	792191	Chrysene-d12	21.633

Hit#	of	2	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine, 2,4-bis(2,2,2-tr...	534	C16H10F12N4O3	302602-84-2	10		
2	Platinum, bis[bis(1,1-dimethylet...	639	C28H46P2Pt	059765-06-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070824\
Data File : BP020863.D
Acq On : 09 Jul 2024 14:01
Operator : MA/JU
Sample : P3084-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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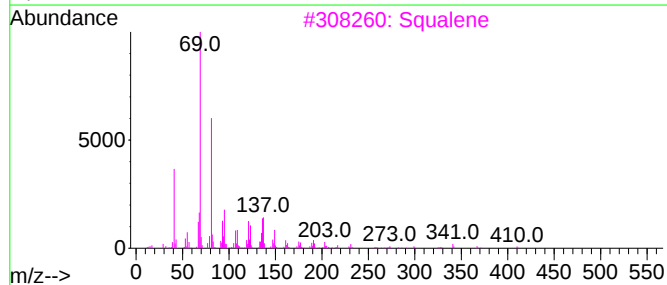
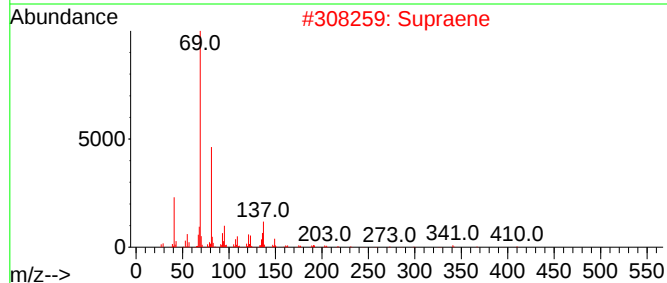
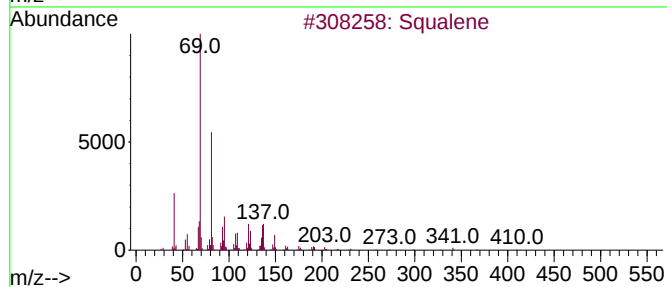
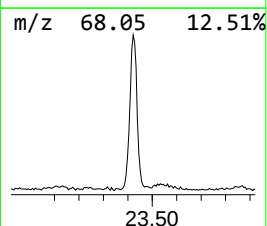
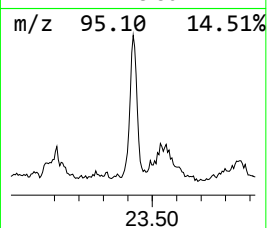
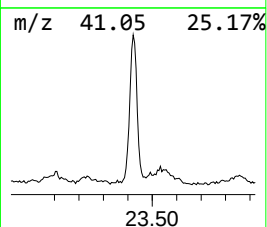
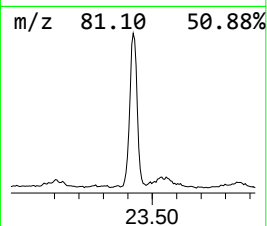
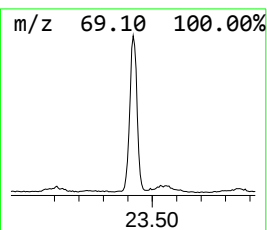
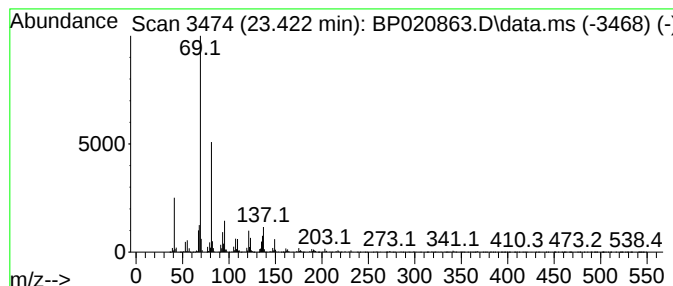
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.422	11.02 ng/ul	1849090	Perylene-d12	24.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	96
2			Supraene	410	C30H50	007683-64-9	91
3			Squalene	410	C30H50	000111-02-4	91
4			Farnesol isomer a	222	C15H26O	1000108-92-4	64
5			trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070824\
Data File : BP020863.D
Acq On : 09 Jul 2024 14:01
Operator : MA/JU
Sample : P3084-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
E1G89

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.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
1-Phenoxypropan...	11.240	2.6	ng/ul	222450	2	10.499	1692750	20.0
n-Hexadecanoic ...	18.122	8.9	ng/ul	1255220	4	17.175	2824260	20.0
Ergost-25-ene-3...	20.563	2.5	ng/ul	359407	5	21.633	2932500	20.0
2-Chloropropio...	21.298	10.6	ng/ul	1546590	5	21.633	2932500	20.0
1-Methyl-4-(1-m...	22.063	2.6	ng/ul	376770	5	21.633	2932500	20.0
unknown-01	22.092	5.4	ng/ul	792191	5	21.633	2932500	20.0
Squalene	23.422	11.0	ng/ul	1849090	6	24.980	3356890	20.0