

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111324\
 Data File : BP023121.D
 Acq On : 15 Nov 2024 02:33
 Operator : RC/JU
 Sample : P4801-12
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 GCPB3

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: BP023121.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	21	25	29	rBV	15568	18502	0.14%	0.036%
2	3.558	93	97	108	rBV	35175	65957	0.49%	0.129%
3	4.352	227	232	242	rBV	18358	29477	0.22%	0.058%
4	6.787	640	646	663	rBV	56563	126022	0.94%	0.247%
5	6.922	663	669	684	rVB	211235	329073	2.46%	0.644%
6	7.122	696	703	716	rBV	243613	421489	3.15%	0.825%
7	7.575	772	780	791	rBV	272899	446946	3.34%	0.874%
8	8.287	895	901	919	rBV	191241	374650	2.80%	0.733%
9	8.722	967	975	992	rBV	274068	493350	3.69%	0.965%
10	8.881	995	1002	1009	rVB3	9506	17040	0.13%	0.033%
11	9.428	1087	1095	1110	rBV	232865	445268	3.33%	0.871%
12	9.975	1181	1188	1212	rBV	302235	665087	4.97%	1.301%
13	10.322	1240	1247	1258	rBV	351567	605575	4.53%	1.185%
14	10.481	1267	1274	1295	rBV	171044	371399	2.78%	0.727%
15	11.581	1457	1461	1469	rVB2	9682	16977	0.13%	0.033%
16	13.598	1797	1804	1822	rBV	696116	1241346	9.28%	2.428%
17	13.840	1838	1845	1846	rBV	12749	17280	0.13%	0.034%
18	13.875	1846	1851	1862	rVB	948843	1271507	9.50%	2.487%
19	14.193	1898	1905	1917	rBV	630205	947425	7.08%	1.853%
20	14.493	1950	1956	1958	rBV2	36814	58874	0.44%	0.115%
21	15.210	2069	2078	2085	rBV	1402365	1831410	13.69%	3.583%
22	15.351	2096	2102	2118	rVV	369781	658596	4.92%	1.288%
23	15.457	2118	2120	2129	rVB8	8454	13761	0.10%	0.027%
24	16.410	2276	2282	2286	rBV8	9961	18903	0.14%	0.037%
25	16.592	2309	2313	2319	rBV3	12093	17824	0.13%	0.035%
26	17.004	2378	2383	2390	rVV	918432	1287031	9.62%	2.518%
27	17.098	2393	2399	2413	rVV	1467679	2118420	15.83%	4.144%
28	17.498	2461	2467	2476	rBV	86883	167839	1.25%	0.328%
29	17.698	2496	2501	2511	rVB	264119	289841	2.17%	0.567%
30	17.869	2524	2530	2537	rVB2	47901	71209	0.53%	0.139%
31	17.957	2537	2545	2570	rBV	2433653	3865853	28.89%	7.563%
32	18.175	2575	2582	2602	rBV	2434478	3946285	29.49%	7.720%
33	18.469	2629	2632	2636	rBV4	12232	18602	0.14%	0.036%
34	18.651	2658	2663	2671	rBV4	36063	59635	0.45%	0.117%
35	19.039	2725	2729	2734	rBV2	22251	33688	0.25%	0.066%
36	19.186	2739	2754	2768	rBV	6782031	13382157	100.00%	26.180%

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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
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37	19.298	2768	2773	2792	rVB	2675619	3623074	27.07%	7.088%
38	19.498	2801	2807	2814	rVB	2259238	3056905	22.84%	5.980%
39	20.310	2942	2945	2950	rBV5	30134	41978	0.31%	0.082%
40	20.416	2958	2963	2970	rBV	116266	204417	1.53%	0.400%
41	21.433	3130	3136	3141	rBV2	1300814	2057357	15.37%	4.025%
42	24.433	3637	3646	3664	rVB	1672759	4005373	29.93%	7.836%
43	24.645	3674	3682	3708	rVB	791701	2382646	17.80%	4.661%

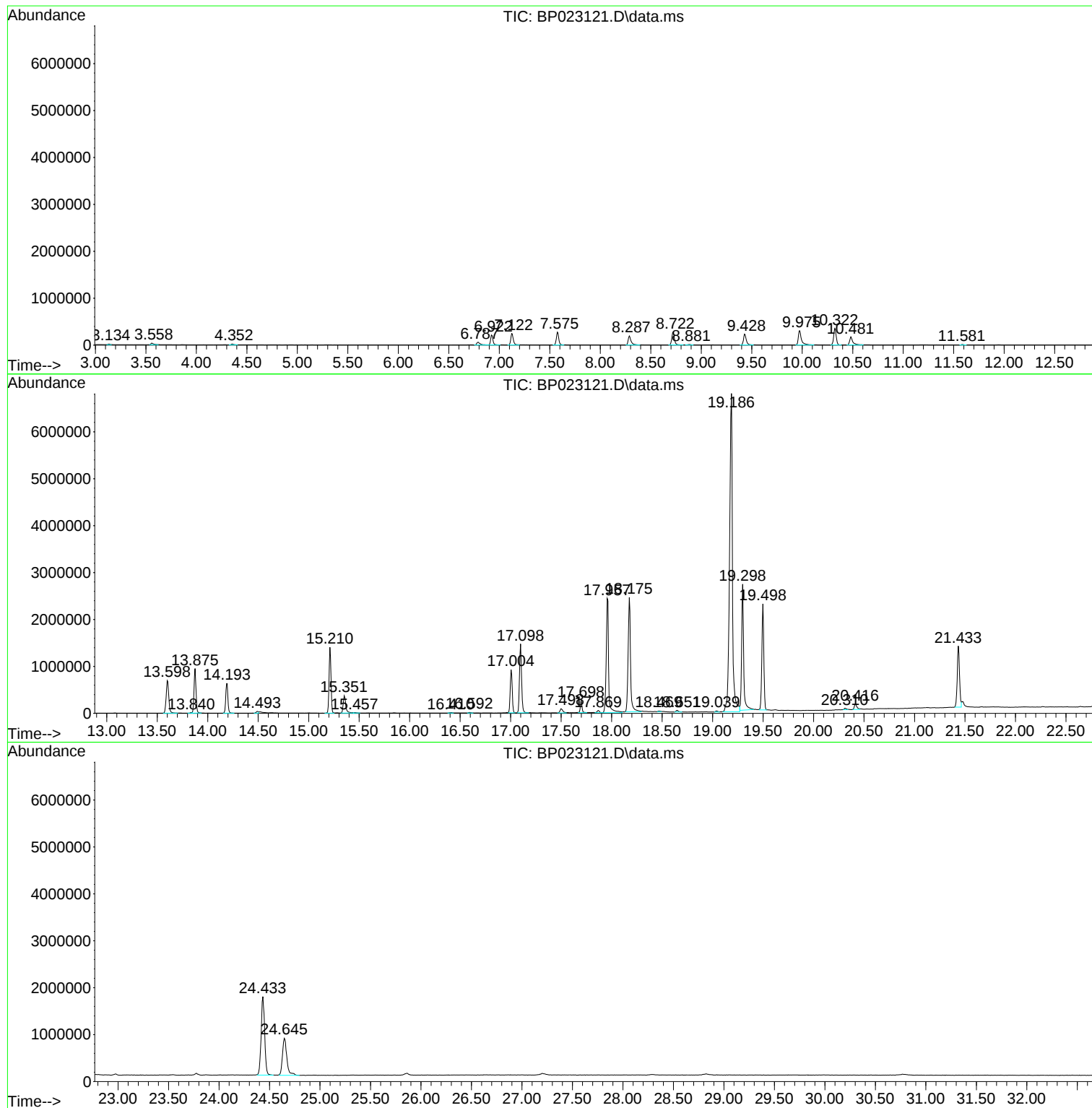
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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



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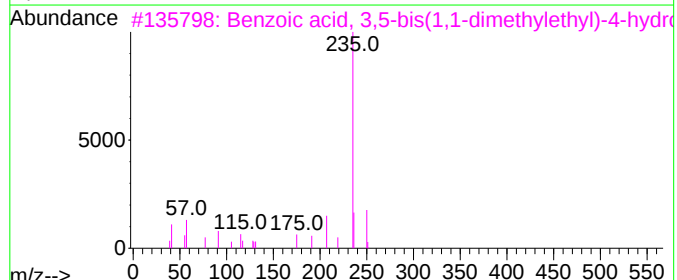
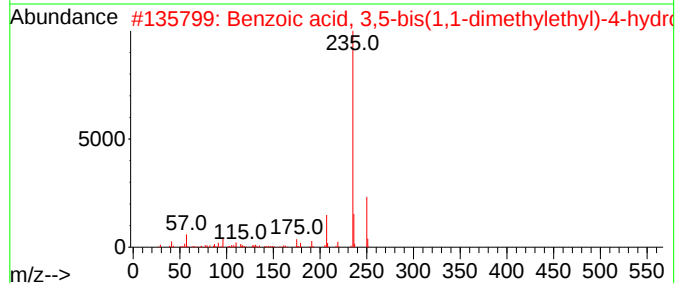
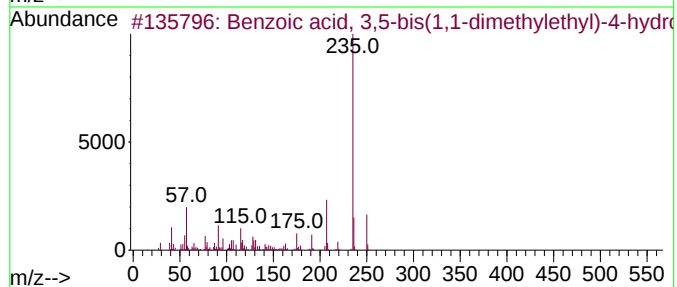
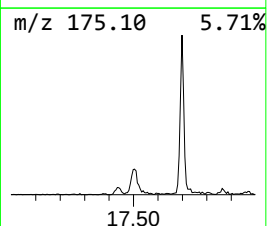
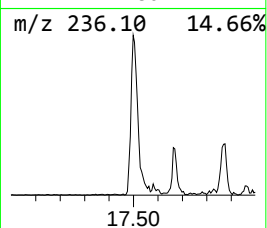
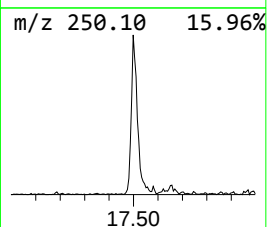
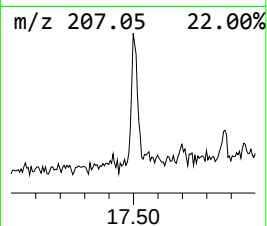
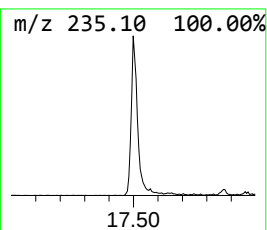
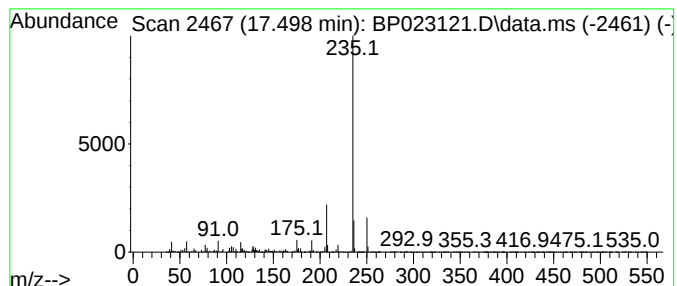
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzoic acid, 3,5-bis(1,1-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.498	2.61 ng/ul	167839	Phenanthrene-d10	17.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	95
2			Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	91
3			Benzoic acid, 3,5-bis(1,1-dimeth...	250	C15H22O3	001421-49-4	70
4			2,5-di-tert-Butyl-1,4-dimethoxyb...	250	C16H26O2	007323-63-9	59
5			3-tert-Butylbenzoic acid, TMS	250	C14H22O2Si	1000507-56-6	59



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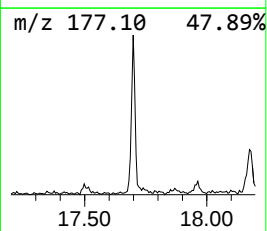
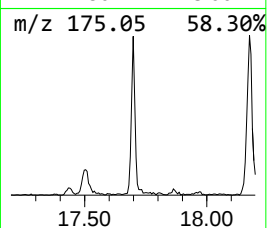
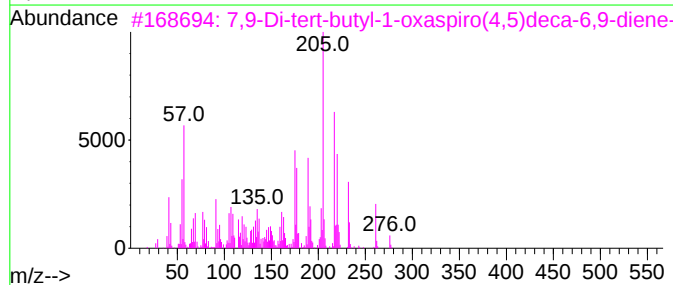
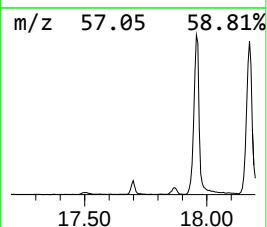
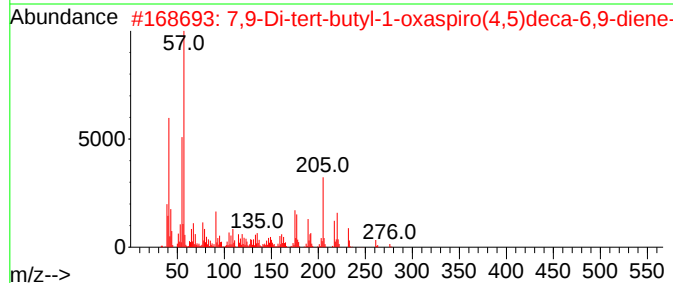
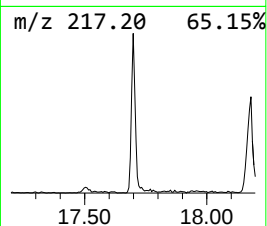
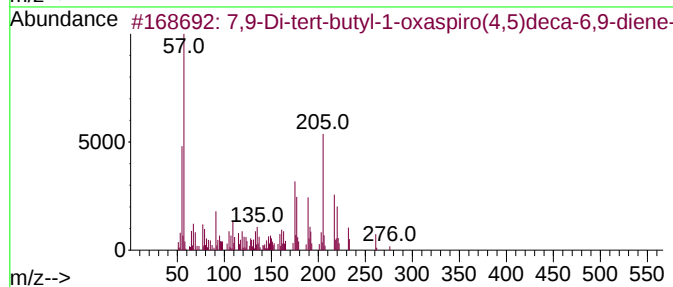
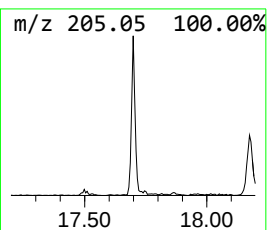
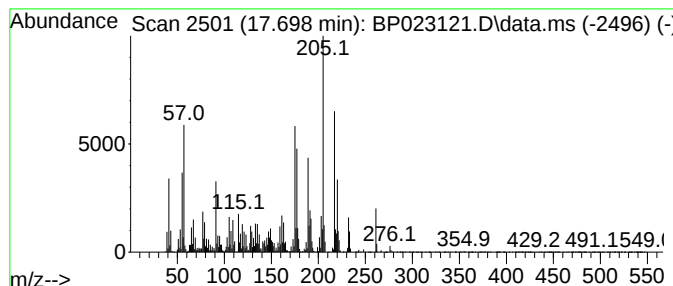
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.698	4.50 ng/ul	289841	Phenanthrene-d10		17.004	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	70
3	7,9-Di-tert-butyl-1-oxaspiro(4,5...		276	C17H24O3	082304-66-3	55
4	Ethanone, 1-(5,6,7,8-tetrahydro-...		220	C14H20O2	071596-88-8	46
5	2,5-di-tert-Butyl-1,4-benzoquinone		220	C14H20O2	002460-77-7	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111324\
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ALS Vial : 45 Sample Multiplier: 1

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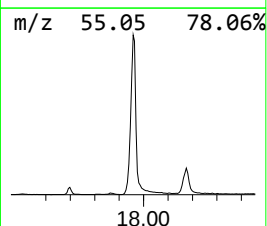
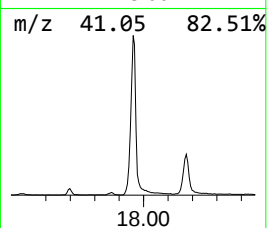
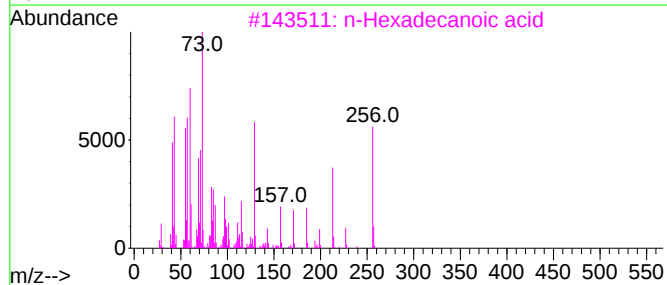
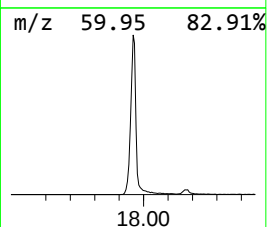
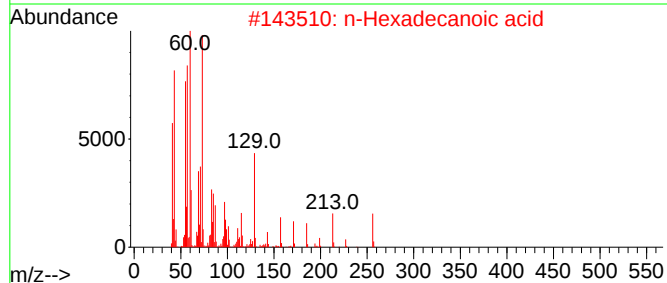
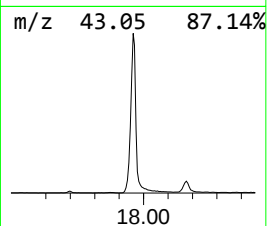
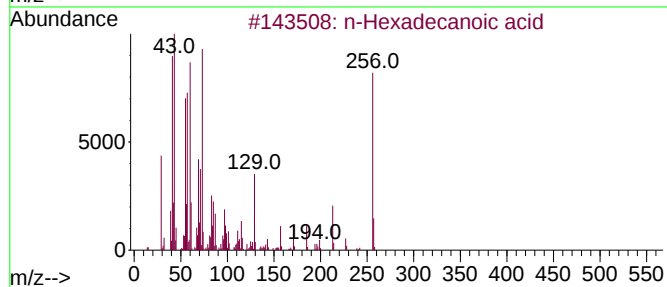
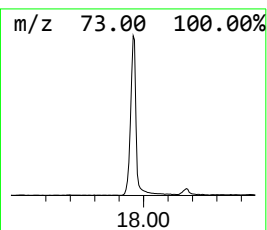
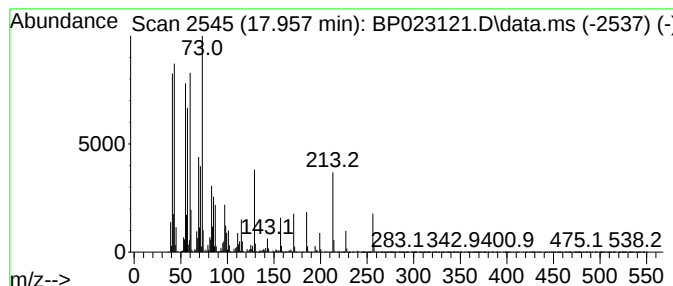
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP110924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.957	60.07 ng/ul	3865850	Phenanthrene-d10	17.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
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	93



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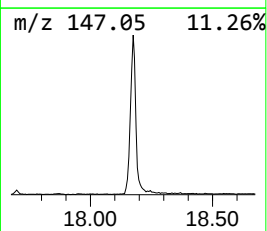
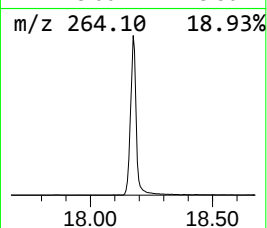
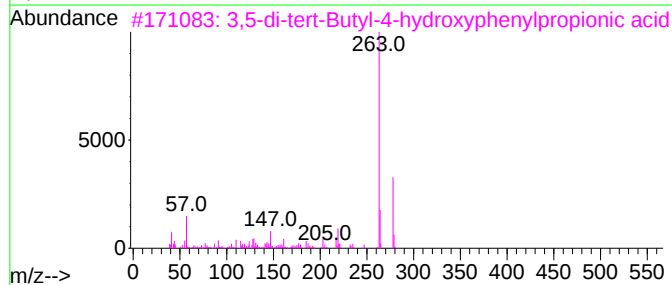
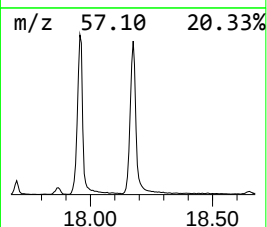
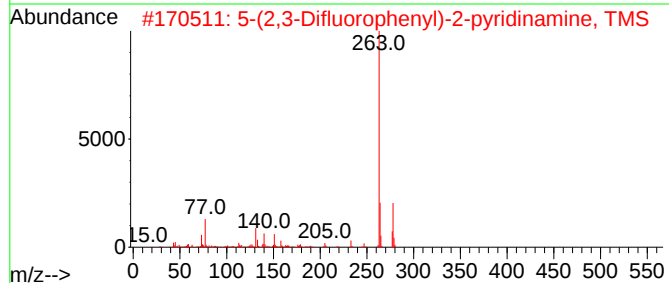
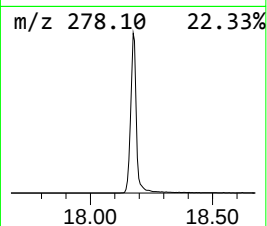
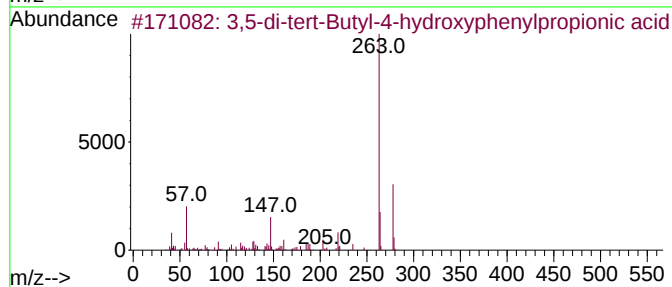
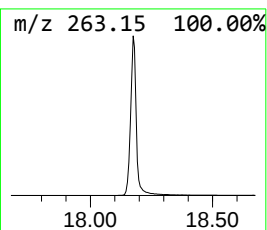
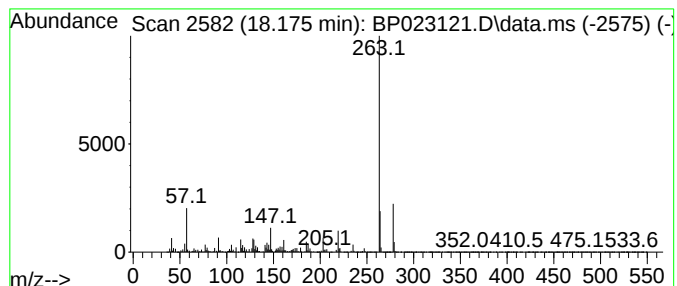
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.175	61.32 ng/ul	3946290	Phenanthrene-d10	17.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	94
2			5-(2,3-Difluorophenyl)-2-pyridin...	278	C14H16F2N2Si	1000504-49-4	72
3			3,5-di-tert-Butyl-4-hydroxypheny...	278	C17H26O3	020170-32-5	62
4			2,6-Bis(tert-butyl)phenol, TMS d...	278	C17H30OSi	010416-73-6	59
5			2,4-Di-tert-butylphenoxytrimethy...	278	C17H30OSi	053925-65-8	58



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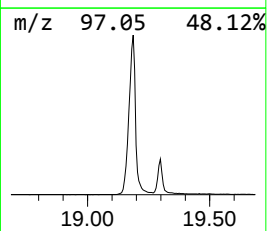
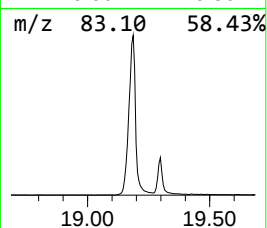
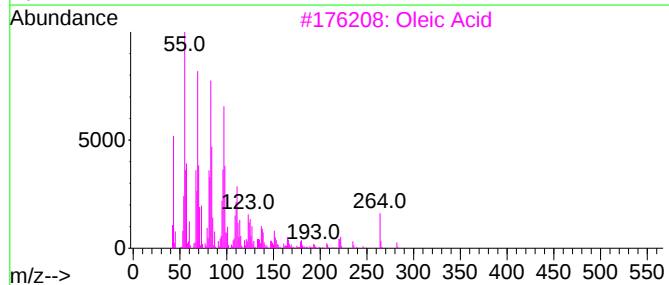
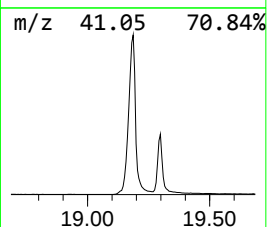
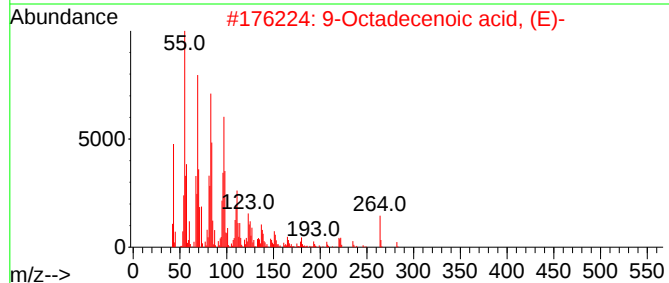
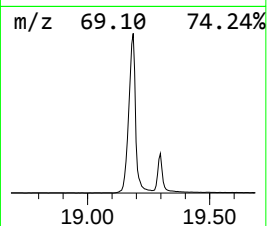
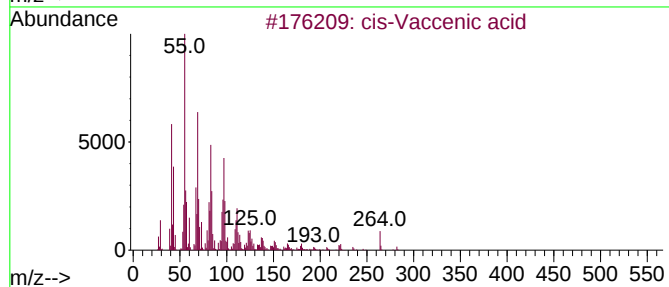
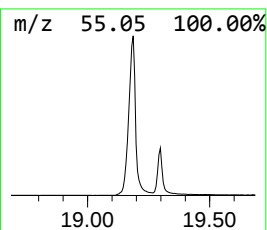
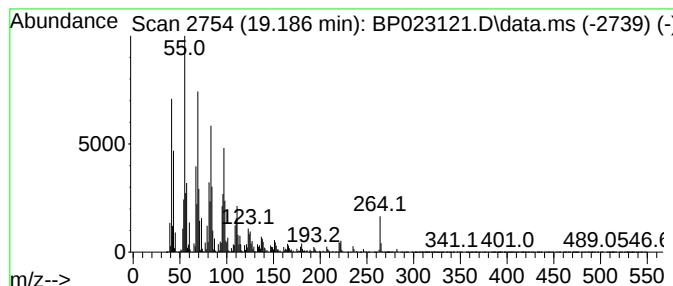
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 cis-Vaccenic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.186	207.95 ng/ul	13382200	Phenanthrene-d10	17.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	99
2			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	97
3			Oleic Acid	282	C18H34O2	000112-80-1	97
4			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	95
5			9-Octadecenoic acid	282	C18H34O2	002027-47-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111324\
Data File : BP023121.D
Acq On : 15 Nov 2024 02:33
Operator : RC/JU
Sample : P4801-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCPB3

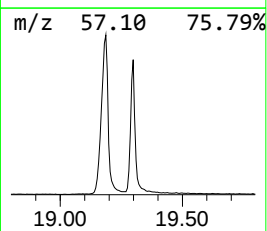
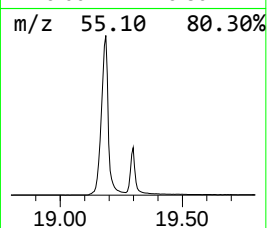
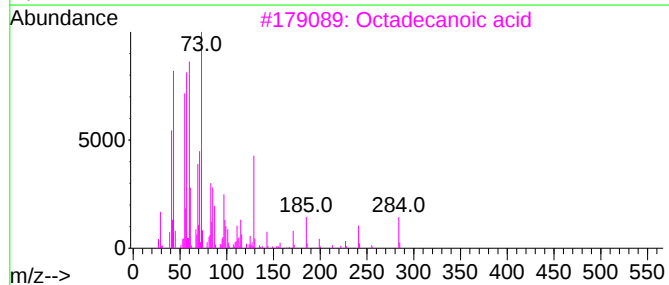
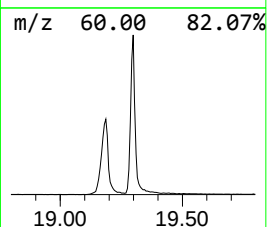
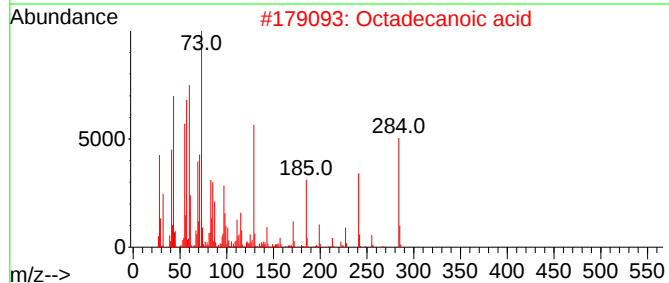
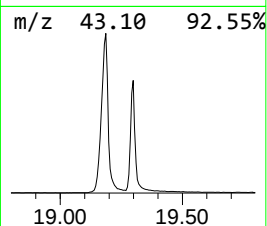
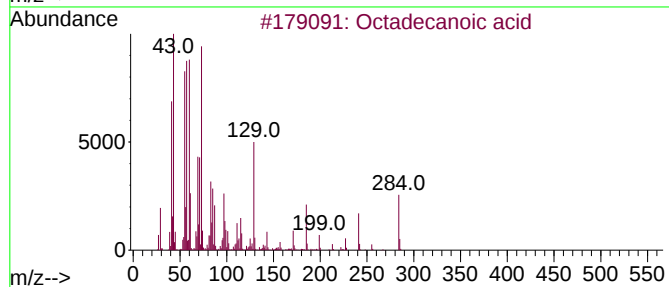
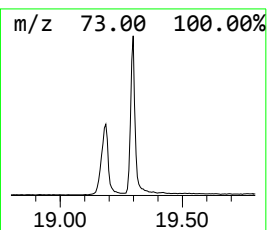
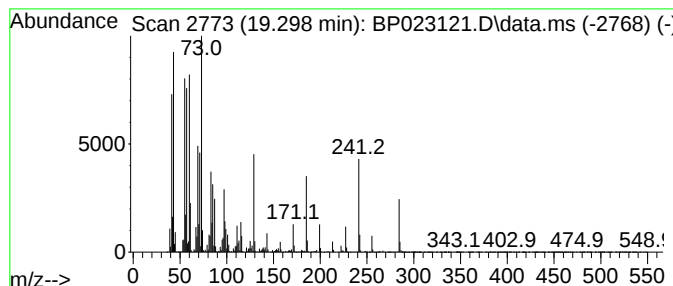
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.298	35.22 ng/ul	3623070	Chrysene-d12	21.433

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	93
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111324\
Data File : BP023121.D
Acq On : 15 Nov 2024 02:33
Operator : RC/JU
Sample : P4801-12
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
GCPB3

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
Benzoic acid, 3...	17.498	2.6	ng/ul	167839	4	17.004	1287030	20.0
7,9-Di-tert-but...	17.698	4.5	ng/ul	289841	4	17.004	1287030	20.0
n-Hexadecanoic ...	17.957	60.1	ng/ul	3865850	4	17.004	1287030	20.0
3,5-di-tert-But...	18.175	61.3	ng/ul	3946290	4	17.004	1287030	20.0
cis-Vaccenic acid	19.186	207.9	ng/ul	13382200	4	17.004	1287030	20.0
Octadecanoic acid	19.298	35.2	ng/ul	3623070	5	21.433	2057360	20.0