

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
 Data File : BP015051.D
 Acq On : 10 May 2023 19:57
 Operator : CG/JU
 Sample : 02591-19
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 JREA7

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-BP050323.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.452	8	11	20	rVB	30297	49136	0.52%	0.059%
2	3.928	91	92	98	rBV4	8870	13565	0.14%	0.016%
3	4.004	102	105	111	rVB	29339	36854	0.39%	0.045%
4	4.128	123	126	133	rVB	14484	24935	0.26%	0.030%
5	4.234	140	144	152	rVB	19948	27685	0.29%	0.033%
6	4.622	205	210	213	rBV6	9245	11247	0.12%	0.014%
7	5.193	302	307	316	rVB2	18458	40513	0.43%	0.049%
8	6.640	548	553	558	rBV2	12041	18512	0.20%	0.022%
9	6.810	573	582	587	rVB3	13331	24428	0.26%	0.030%
10	7.134	632	637	641	rBV3	10705	22937	0.24%	0.028%
11	7.298	656	665	675	rBV	503993	845264	8.93%	1.021%
12	7.469	685	694	706	rVB	425972	694594	7.34%	0.839%
13	7.675	722	729	739	rBV	534282	849014	8.97%	1.026%
14	7.757	739	743	747	rVB3	9452	12130	0.13%	0.015%
15	8.151	802	810	819	rBV	1017540	1626570	17.19%	1.966%
16	8.863	920	931	941	rBV	615828	1042371	11.02%	1.260%
17	8.981	945	951	961	rVB	81500	135803	1.44%	0.164%
18	9.322	1003	1009	1021	rVV	482315	819703	8.66%	0.991%
19	9.481	1031	1036	1040	rVB8	8066	12581	0.13%	0.015%
20	9.722	1072	1077	1082	rBV2	11313	18178	0.19%	0.022%
21	10.057	1125	1134	1144	rBV	393695	681260	7.20%	0.823%
22	10.204	1154	1159	1166	rBV2	19964	40475	0.43%	0.049%
23	10.275	1166	1171	1180	rVB6	12987	30223	0.32%	0.037%
24	10.416	1186	1195	1201	rVB2	12744	27121	0.29%	0.033%
25	10.598	1217	1226	1243	rBV	646181	1111302	11.75%	1.343%
26	10.981	1282	1291	1298	rBV	1431738	2412652	25.50%	2.916%
27	11.034	1298	1300	1306	rVV2	29451	41725	0.44%	0.050%
28	11.116	1308	1314	1331	rVV	252348	498212	5.27%	0.602%
29	11.510	1376	1381	1392	rBV2	15625	35104	0.37%	0.042%
30	11.763	1415	1424	1433	rBV6	18391	44701	0.47%	0.054%
31	11.898	1440	1447	1453	rBV10	14651	26941	0.28%	0.033%
32	12.381	1523	1529	1533	rVB8	5335	9578	0.10%	0.012%
33	12.469	1538	1544	1550	rBV5	11167	24365	0.26%	0.029%
34	12.557	1554	1559	1564	rVB2	12444	20327	0.21%	0.025%
35	12.651	1567	1575	1586	rBV3	44230	134288	1.42%	0.162%
36	12.775	1592	1596	1601	rVB2	15871	26663	0.28%	0.032%

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37	13.333	1685	1691	1696	rVB9	7387	12926	0.14%	0.016%
38	13.604	1725	1737	1740	rBV6	11437	30454	0.32%	0.037%
39	13.710	1750	1755	1762	rBV	48660	79366	0.84%	0.096%
40	13.775	1762	1766	1770	rVV7	9038	14661	0.15%	0.018%
41	13.822	1770	1774	1782	rVB7	7773	18194	0.19%	0.022%
42	14.110	1818	1823	1828	rVB9	6965	12683	0.13%	0.015%
43	14.192	1828	1837	1844	rBV	1189138	1628299	17.21%	1.968%
44	14.316	1854	1858	1861	rVB5	8016	11788	0.12%	0.014%
45	14.486	1880	1887	1899	rBV	1403942	2052078	21.69%	2.480%
46	14.639	1909	1913	1923	rVB	39743	69992	0.74%	0.085%
47	14.792	1932	1939	1947	rBV	2087810	3073669	32.49%	3.714%
48	14.980	1965	1971	1978	rBV	300718	498266	5.27%	0.602%
49	15.139	1993	1998	2002	rBV5	16234	24604	0.26%	0.030%
50	15.186	2002	2006	2011	rBV4	28615	42108	0.45%	0.051%
51	15.286	2019	2023	2027	rVB	23030	32229	0.34%	0.039%
52	15.339	2027	2032	2035	rBV6	7724	12245	0.13%	0.015%
53	15.780	2101	2107	2114	rBV	1676601	2431572	25.70%	2.938%
54	15.898	2122	2127	2133	rBV	226204	321752	3.40%	0.389%
55	16.145	2163	2169	2176	rVB	229280	324626	3.43%	0.392%
56	16.480	2224	2226	2228	rBV3	10291	10231	0.11%	0.012%
57	16.710	2262	2265	2270	rVB2	30534	39151	0.41%	0.047%
58	16.916	2297	2300	2309	rBV6	41123	62484	0.66%	0.076%
59	17.192	2342	2347	2355	rBV2	172920	252124	2.67%	0.305%
60	17.421	2382	2386	2391	rBV	47099	70643	0.75%	0.085%
61	17.486	2394	2397	2400	rBV3	25007	30130	0.32%	0.036%
62	17.545	2401	2407	2413	rBV	2216050	3202400	33.85%	3.870%
63	17.645	2418	2424	2429	rBV	1594564	2264144	23.93%	2.736%
64	18.292	2530	2534	2538	rVB3	64436	89097	0.94%	0.108%
65	18.345	2540	2543	2547	rBV3	70770	91230	0.96%	0.110%
66	18.404	2548	2553	2563	rBV	917383	1400584	14.80%	1.693%
67	18.527	2571	2574	2579	rVB4	92680	120807	1.28%	0.146%
68	18.792	2615	2619	2626	rVB	409418	555162	5.87%	0.671%
69	18.968	2645	2649	2656	rBV	569368	757602	8.01%	0.916%
70	19.110	2670	2673	2677	rVB	122282	145580	1.54%	0.176%
71	19.286	2700	2703	2709	rVB	138195	157018	1.66%	0.190%
72	19.621	2757	2760	2765	rBV2	249959	367154	3.88%	0.444%
73	19.862	2796	2801	2808	rVB	1534428	2066850	21.85%	2.498%
74	20.286	2870	2873	2877	rVB	199234	231822	2.45%	0.280%
75	20.333	2877	2881	2883	rBV	371558	490672	5.19%	0.593%
76	20.674	2936	2939	2943	rBV	259939	310461	3.28%	0.375%

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77	21.298	3040	3045	3055	rVB	5670859	7923422	83.76%	9.575%
78	21.615	3094	3099	3112	rBV2	4916274	8362640	88.40%	10.106%
79	21.721	3114	3117	3121	rVV	597281	749095	7.92%	0.905%
80	22.268	3205	3210	3222	rVB	5986951	9309069	98.40%	11.250%
81	22.651	3268	3275	3287	rBV2	4605710	9460236	100.00%	11.432%
82	23.380	3396	3399	3404	rBV	461296	750627	7.93%	0.907%
83	23.445	3406	3410	3422	rVB	933509	1943864	20.55%	2.349%
84	24.045	3507	3512	3526	rVB2	967705	2187121	23.12%	2.643%
85	24.215	3536	3541	3549	rVB	1211778	2477652	26.19%	2.994%
86	27.974	4173	4180	4195	rVB3	1291101	4687531	49.55%	5.665%

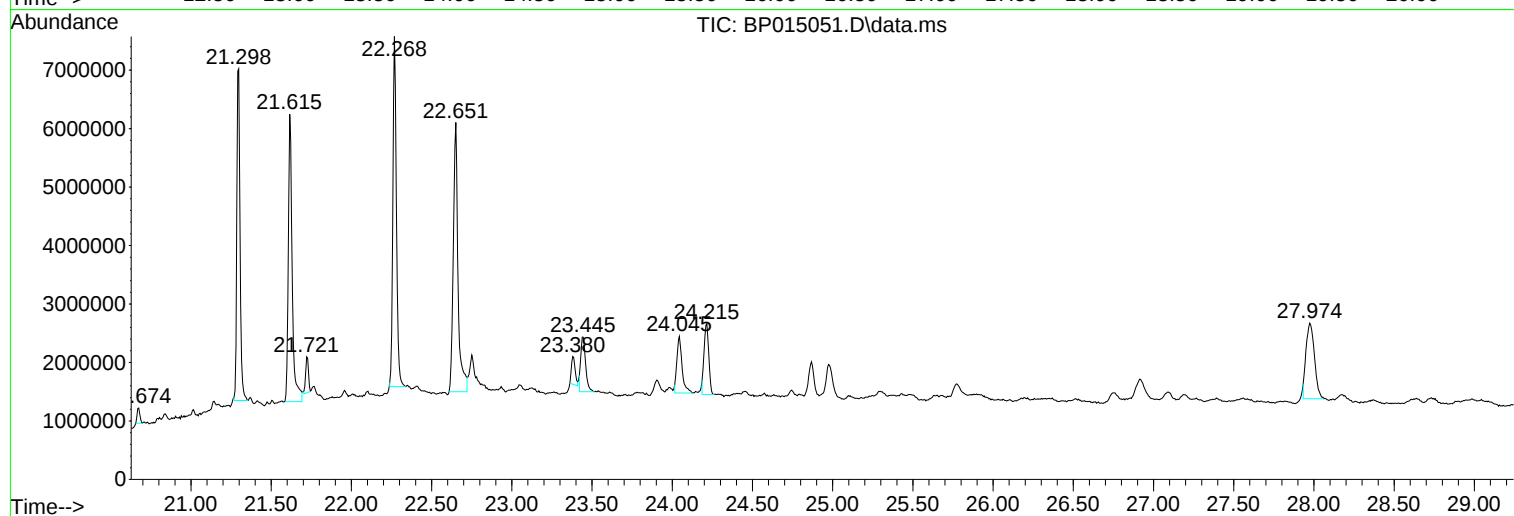
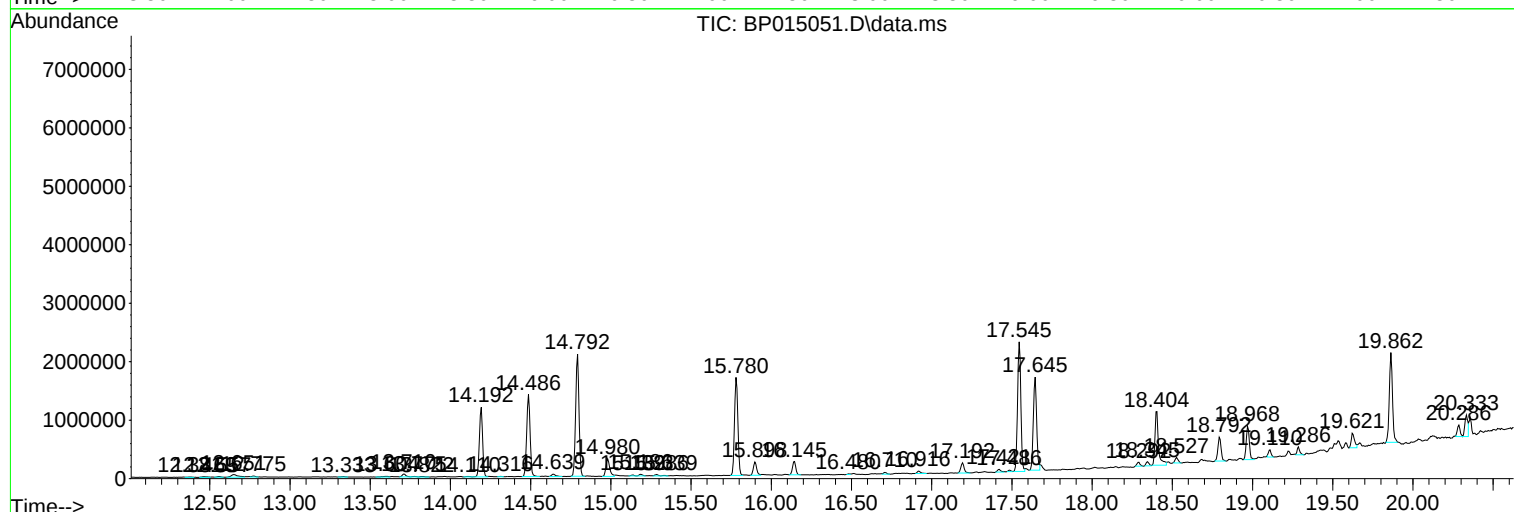
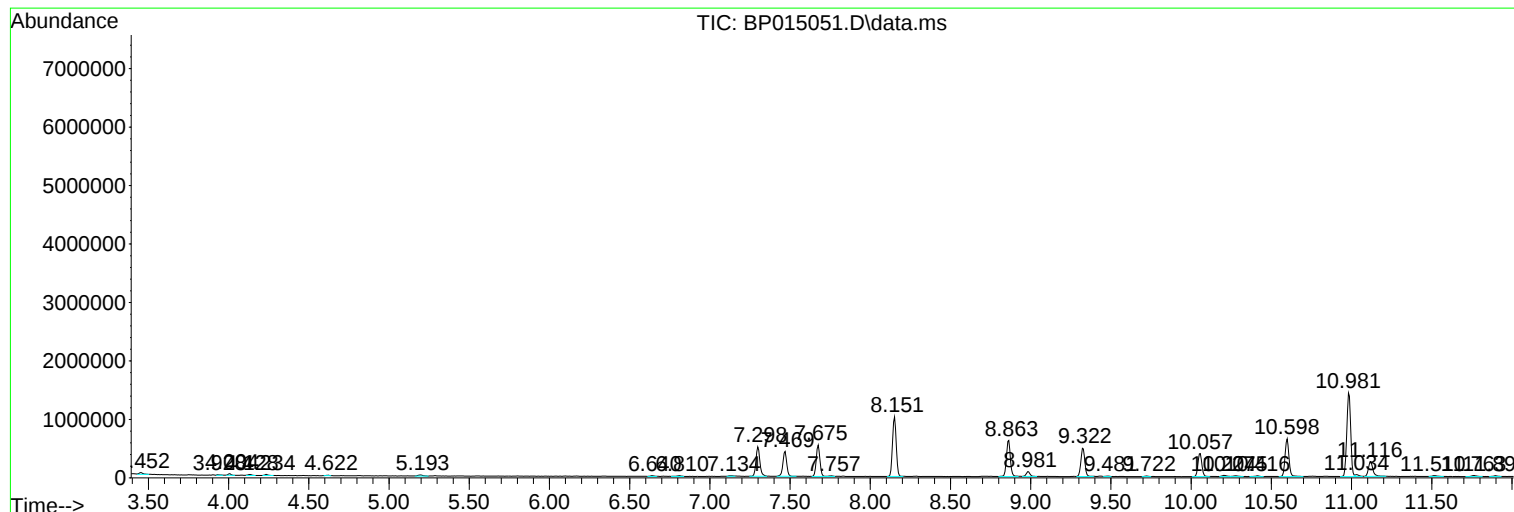
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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



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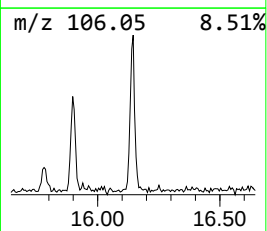
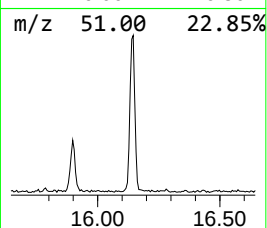
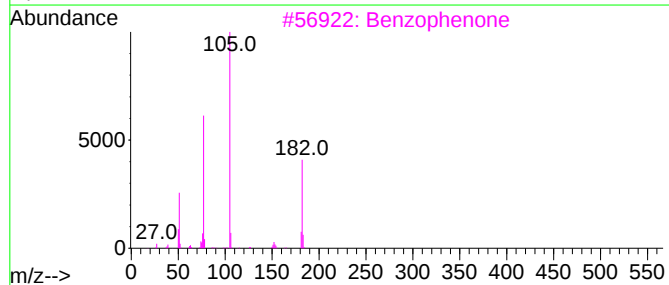
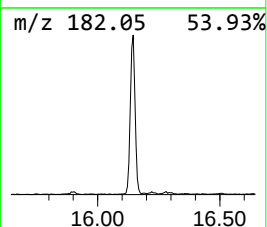
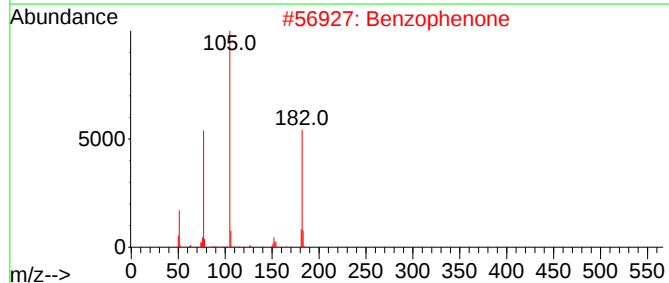
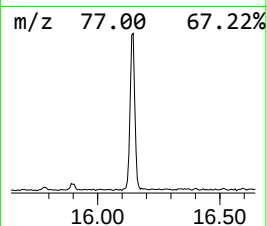
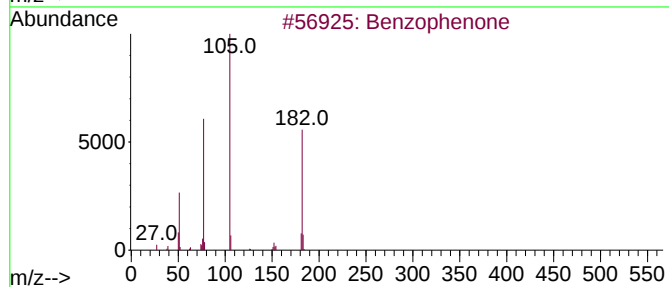
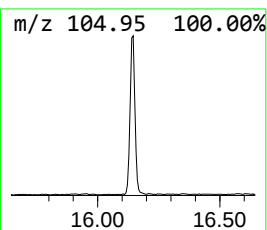
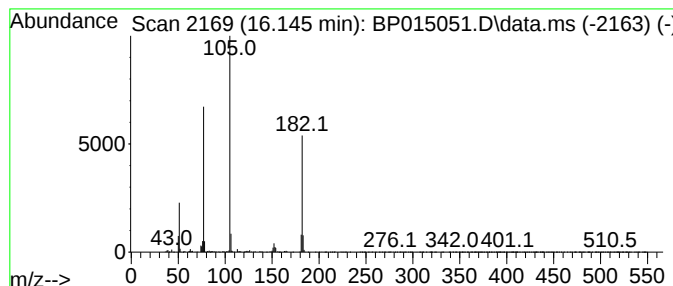
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	2.11 ng/ul	324626	Acenaphthene-d10	14.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzophenone	182	C13H10O	000119-61-9	95
3			Benzophenone	182	C13H10O	000119-61-9	94
4			Benzophenone	182	C13H10O	000119-61-9	93
5			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	64



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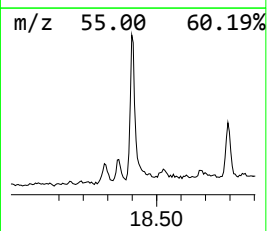
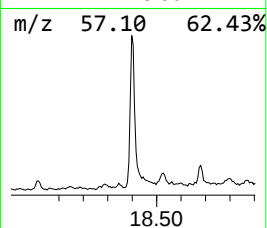
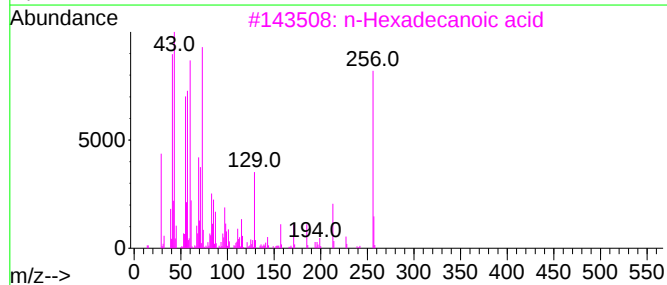
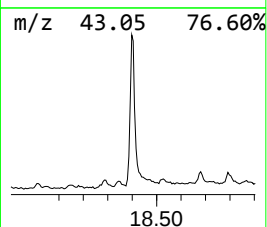
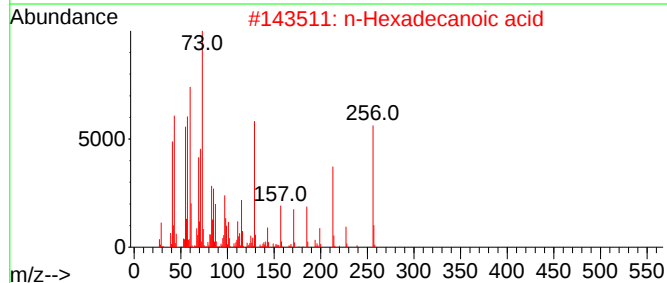
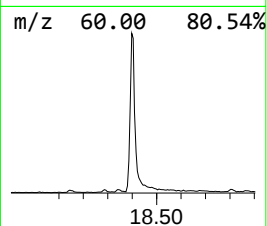
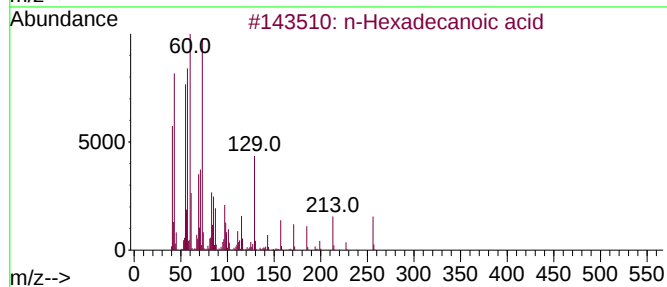
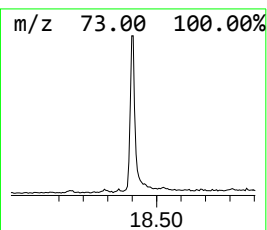
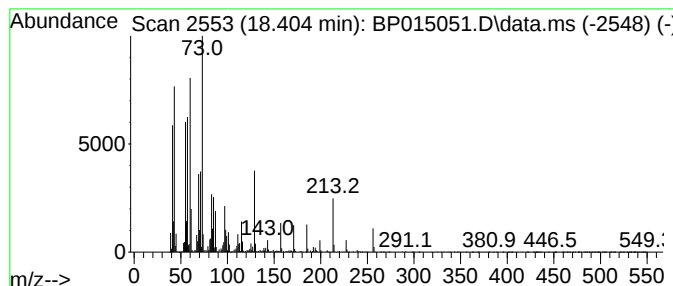
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	8.75 ng/ul	1400580	Phenanthrene-d10	17.545

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	99
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	93



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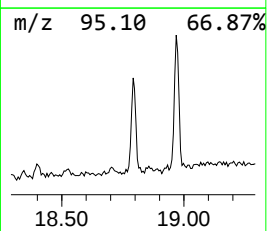
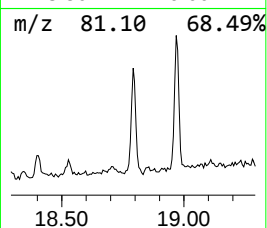
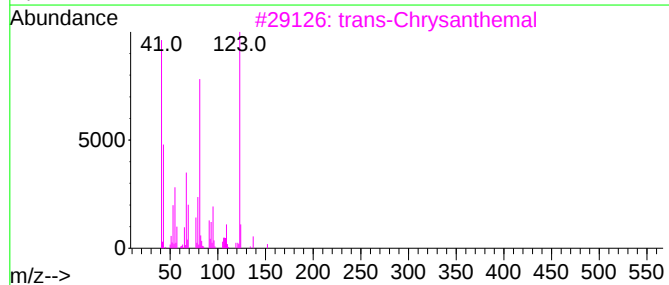
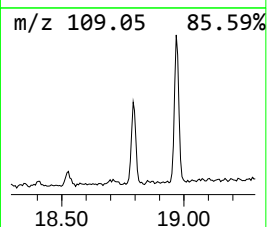
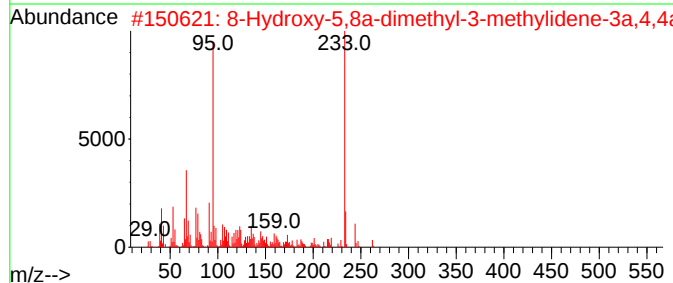
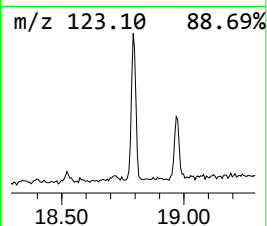
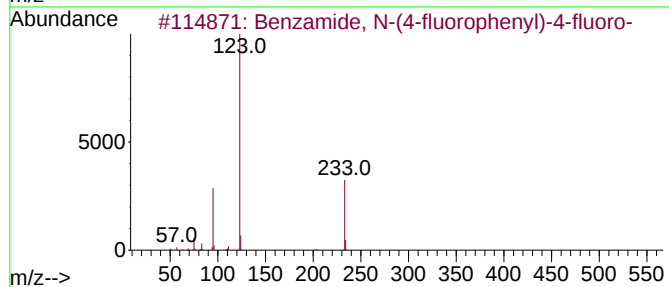
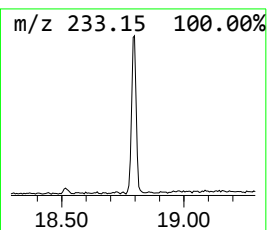
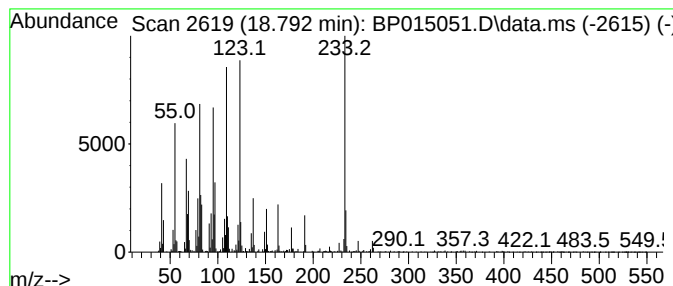
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.792	3.47 ng/ul	555162	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-(4-fluorophenyl)-4-...	233	C13H9F2NO	1000307-10-1	43
2			8-Hydroxy-5,8a-dimethyl-3-methyl...	262	C15H18O4	1379770-19-0	30
3			trans-Chrysanthemal	152	C10H16O	020104-05-6	25
4			4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	18
5			1,2,3-Trimethyl-cyclopent-2-enec...	138	C9H14O	1000190-18-1	18



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ClientSampleId :
JREA7

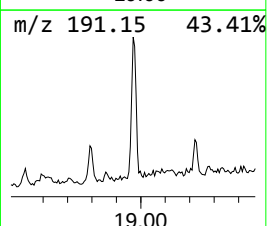
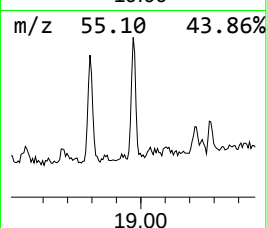
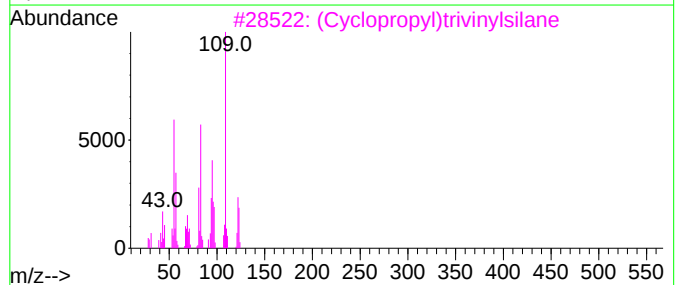
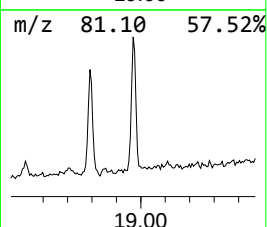
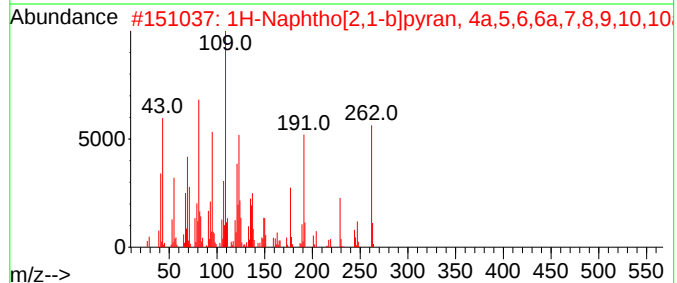
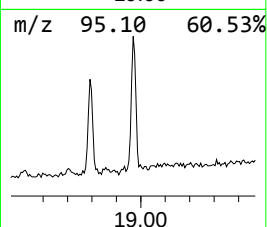
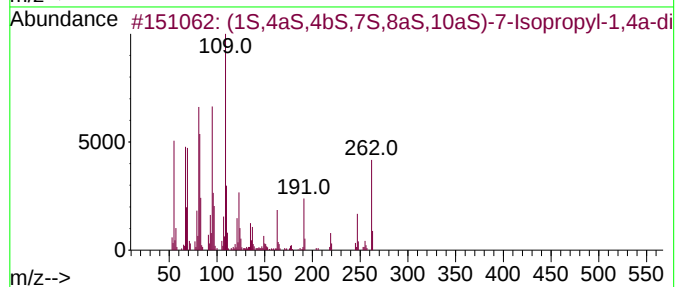
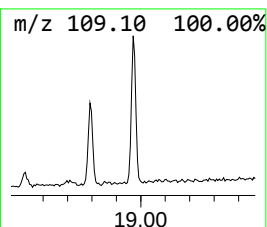
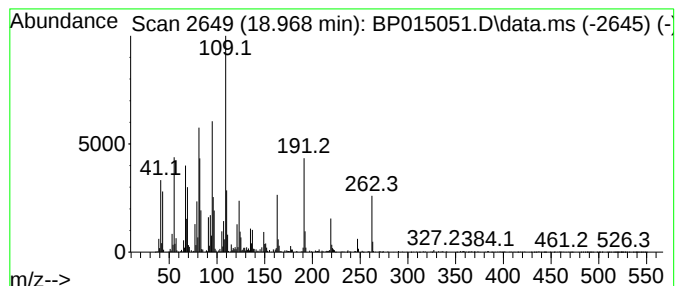
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (1S,4aS,4bS,7S,8aS,10aS)-7-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.968	4.73 ng/ul	757602	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	93
2			1H-Naphtho[2,1-b]pyran, 4a,5,6,6...	262	C18H30O	005153-92-4	46
3			(Cyclopropyl)trivinylsilane	150	C9H14Si	1000109-93-8	38
4			3,6-Octadienal, 3,7-dimethyl-	152	C10H16O	055722-59-3	35
5			(1S,4aS,4bS,7S,8aS,10aS)-7-Isopr...	262	C19H34	002221-95-6	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015051.D
Acq On : 10 May 2023 19:57
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREA7

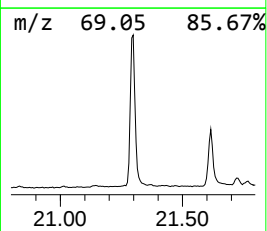
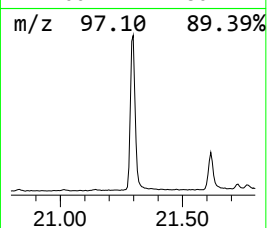
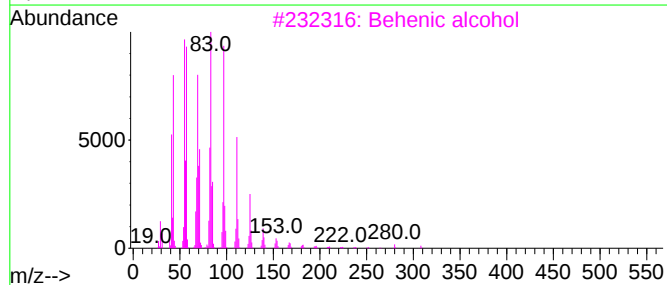
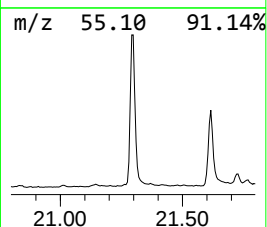
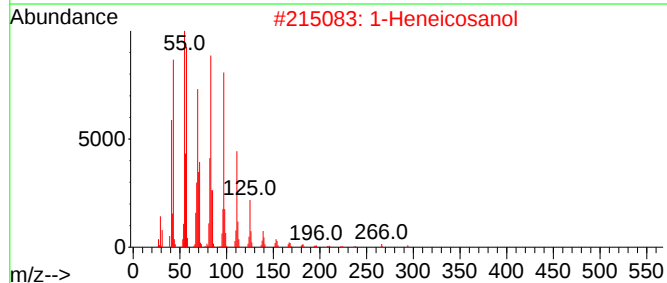
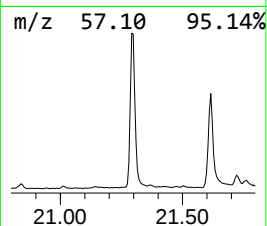
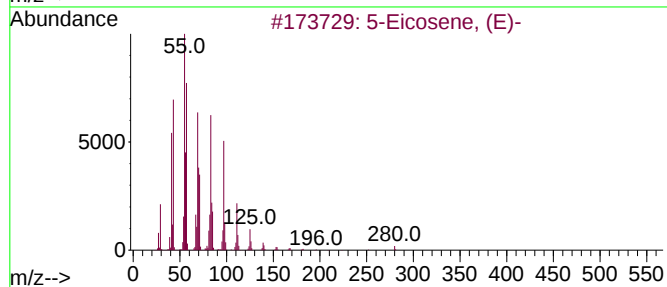
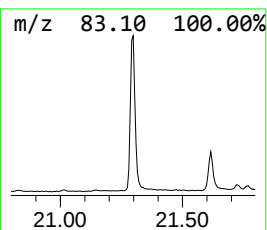
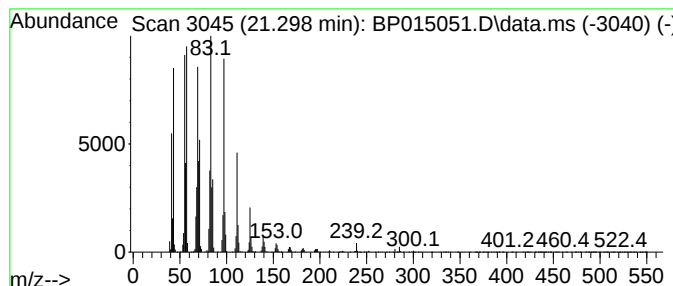
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.298	18.95 ng/ul	7923420	Chrysene-d12	21.627

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Heneicosanol		312	C21H44O	015594-90-8	95
3	Behenic alcohol		326	C22H46O	000661-19-8	94
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	94
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015051.D
Acq On : 10 May 2023 19:57
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

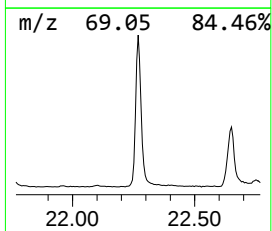
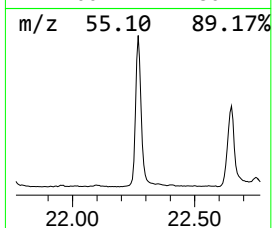
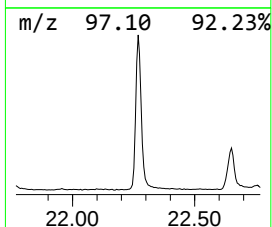
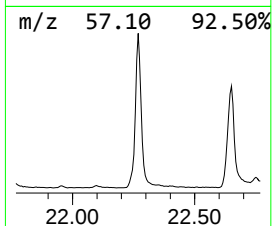
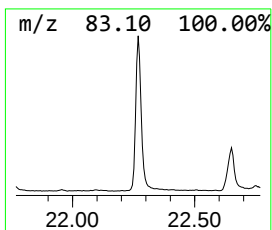
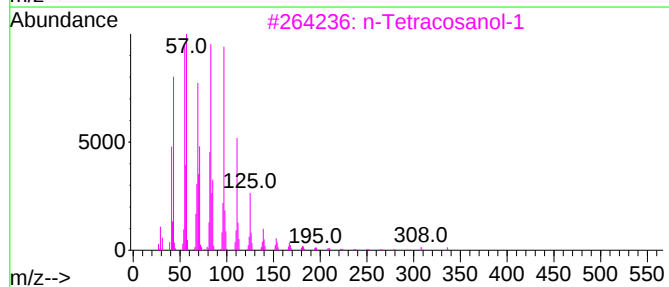
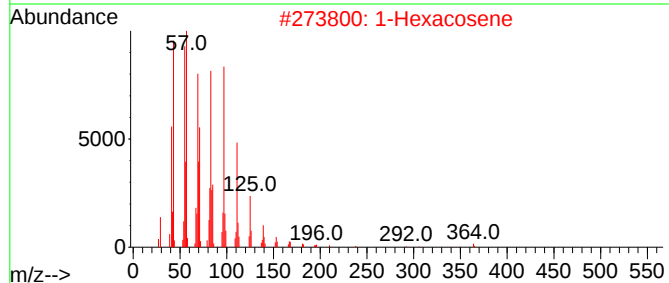
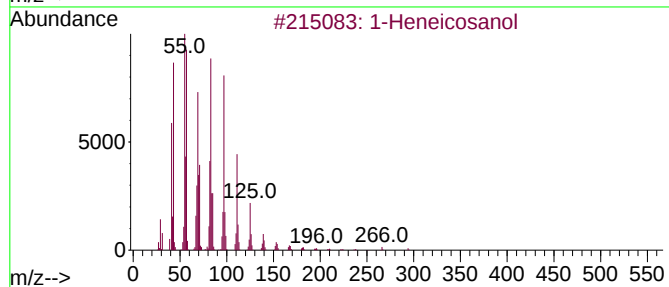
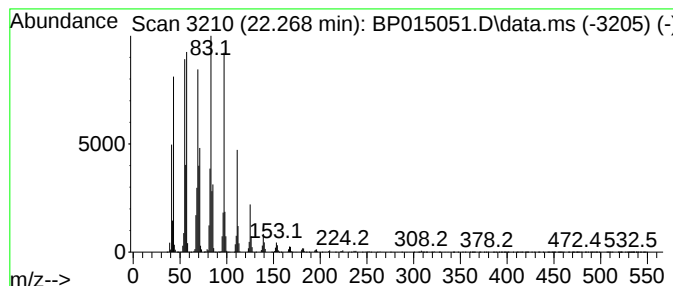
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.268	22.26 ng/ul	9309070	Chrysene-d12	21.627	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015051.D
Acq On : 10 May 2023 19:57
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREA7

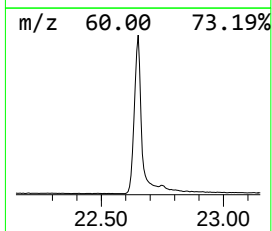
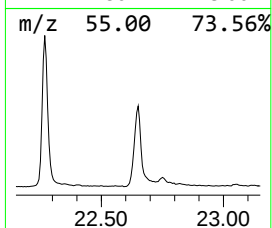
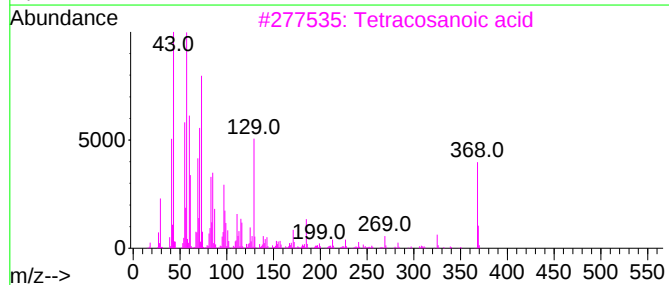
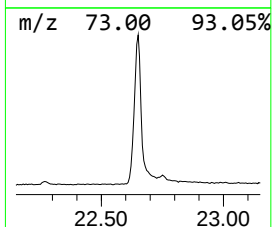
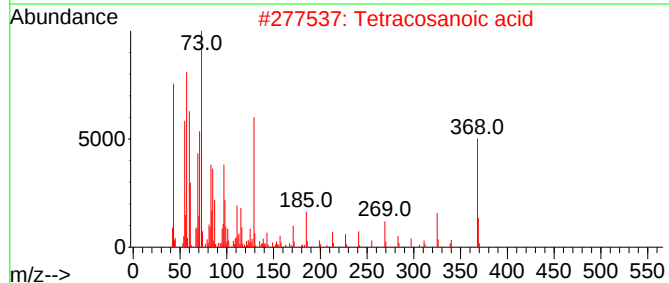
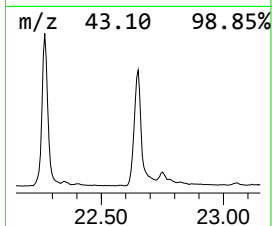
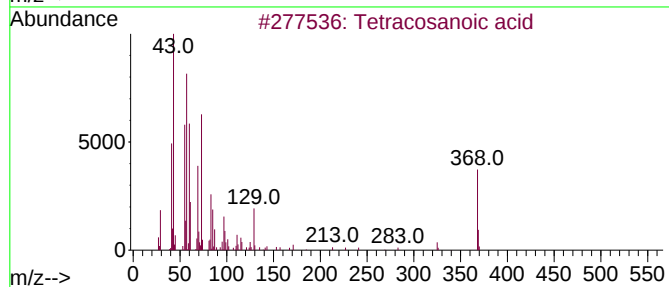
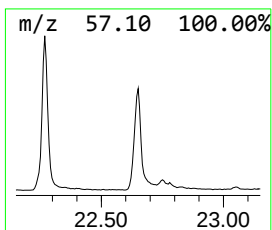
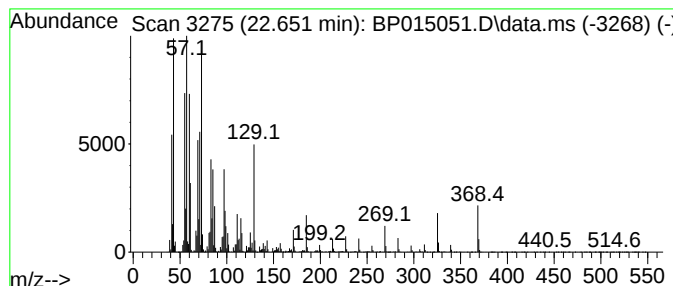
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Tetracosanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.651	22.63 ng/ul	9460240	Chrysene-d12	21.627

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosanoic acid	368	C24H48O2	000557-59-5	99
2			Tetracosanoic acid	368	C24H48O2	000557-59-5	97
3			Tetracosanoic acid	368	C24H48O2	000557-59-5	96
4			Heneicosanoic acid, isopropyl ester	368	C24H48O2	1000405-13-6	64
5			Octadecanoic acid	284	C18H36O2	000057-11-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015051.D
Acq On : 10 May 2023 19:57
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

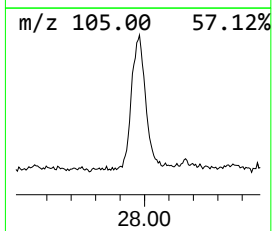
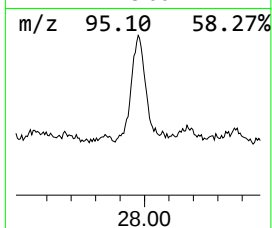
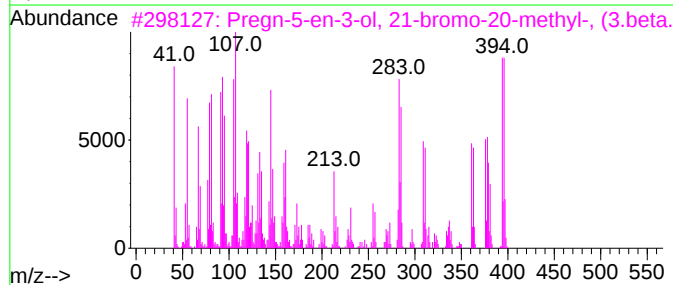
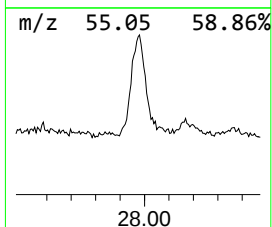
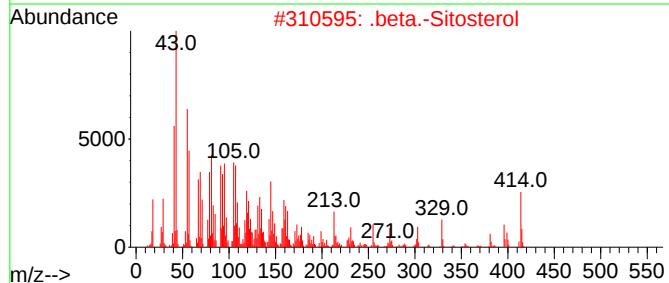
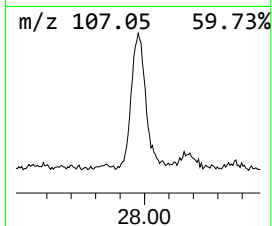
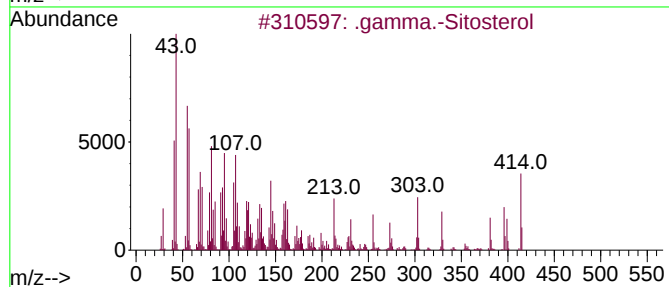
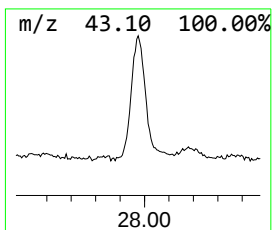
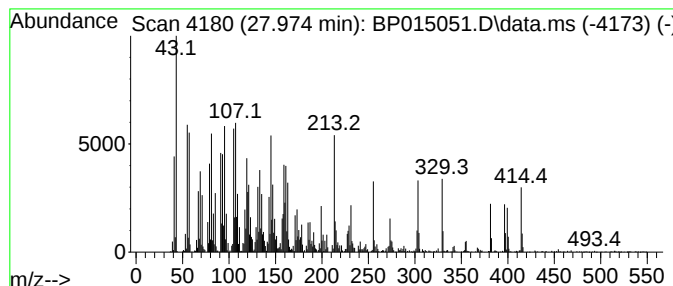
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
27.974	37.84 ng/ul	4687530	Perylene-d12	24.215	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	90
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	74
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	53
5	.beta.-Sitosterol	414	C29H50O	000083-46-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051023\
Data File : BP015051.D
Acq On : 10 May 2023 19:57
Operator : CG/JU
Sample : 02591-19
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
JREA7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP050323.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	16.145	2.1	ng/ul	324626	3	14.792	3073670	20.0
n-Hexadecanoic ...	18.404	8.8	ng/ul	1400580	4	17.545	3202400	20.0
unknown-01	18.792	3.5	ng/ul	555162	4	17.545	3202400	20.0
(1S,4aS,4bS,7S,...	18.968	4.7	ng/ul	757602	4	17.545	3202400	20.0
(DEL) Alkane: S...	21.298	18.9	ng/ul	7923420	5	21.627	8362640	20.0
1-Heneicosanol	22.268	22.3	ng/ul	9309070	5	21.627	8362640	20.0
Tetracosanoic acid	22.651	22.6	ng/ul	9460240	5	21.627	8362640	20.0
.gamma.-Sitosterol	27.974	37.8	ng/ul	4687530	6	24.215	2477650	20.0