

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
 Data File : BP018782.D
 Acq On : 12 Dec 2023 23:40
 Operator : MA/JU
 Sample : 05646-05
 Misc :
 ALS Vial : 61 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 C0AY1

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-BP120123.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP018782.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.164	8	13	19	rVB7	8088	16394	0.44%	0.038%
2	3.264	27	30	36	rVB	24468	32236	0.86%	0.074%
3	3.699	102	104	111	rVB5	13470	15808	0.42%	0.036%
4	3.793	116	120	127	rBV2	38080	53719	1.43%	0.124%
5	3.863	130	132	136	rVV3	7648	11152	0.30%	0.026%
6	3.916	137	141	147	rVB	30343	45135	1.20%	0.104%
7	4.016	153	158	161	rBV	17538	26220	0.70%	0.061%
8	4.181	182	186	190	rVB6	8028	10842	0.29%	0.025%
9	4.240	192	196	201	rBV	43837	55469	1.48%	0.128%
10	4.516	241	243	248	rBV4	6265	11556	0.31%	0.027%
11	4.569	248	252	256	rVV5	9570	13373	0.36%	0.031%
12	4.658	262	267	273	rVB2	25241	34837	0.93%	0.080%
13	4.840	292	298	303	rBV10	4715	10280	0.27%	0.024%
14	4.940	310	315	324	rVB	28766	51657	1.37%	0.119%
15	5.040	328	332	338	rBV3	12086	17303	0.46%	0.040%
16	5.146	346	350	354	rVB4	9252	11913	0.32%	0.027%
17	5.822	459	465	473	rBV	22141	38626	1.03%	0.089%
18	7.005	656	666	683	rVB3	376408	917804	24.43%	2.119%
19	7.175	689	695	705	rVB	331269	501546	13.35%	1.158%
20	7.369	721	728	737	rBV	396705	623146	16.58%	1.438%
21	7.463	740	744	749	rVB6	8462	11944	0.32%	0.028%
22	7.840	799	808	815	rBV	700680	1106639	29.45%	2.555%
23	7.904	815	819	827	rVB4	10383	19799	0.53%	0.046%
24	8.087	843	850	854	rBV10	10612	24460	0.65%	0.056%
25	8.293	878	885	890	rVB2	7018	11114	0.30%	0.026%
26	8.551	922	929	937	rBV	354722	579572	15.42%	1.338%
27	8.663	941	948	959	rVV	470123	745945	19.85%	1.722%
28	8.787	962	969	977	rVV	41413	79660	2.12%	0.184%
29	8.999	997	1005	1012	rBV	381668	597122	15.89%	1.378%
30	9.110	1019	1024	1029	rVB	16417	23734	0.63%	0.055%
31	9.163	1029	1033	1041	rVB8	8325	13779	0.37%	0.032%
32	9.240	1041	1046	1052	rBV9	7964	14644	0.39%	0.034%
33	9.716	1118	1127	1134	rBV	278293	459392	12.23%	1.060%
34	9.910	1147	1160	1167	rBV	189540	475241	12.65%	1.097%
35	10.081	1182	1189	1199	rVB	98918	171345	4.56%	0.396%
36	10.198	1203	1209	1212	rBV3	7583	12790	0.34%	0.030%

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Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
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37	10.257	1212	1219	1233	rVV	468680	800029	21.29%	1.847%
38	10.634	1275	1283	1290	rBV	889884	1491440	39.69%	3.443%
39	10.775	1300	1307	1321	rBV	112086	226506	6.03%	0.523%
40	11.175	1369	1375	1390	rBV2	48764	107783	2.87%	0.249%

41	11.422	1411	1417	1426	rBV	47253	89641	2.39%	0.207%
42	11.557	1435	1440	1445	rBV9	5675	10901	0.29%	0.025%
43	11.669	1454	1459	1466	rVB	10083	14728	0.39%	0.034%
44	11.998	1508	1515	1520	rBV2	20088	31517	0.84%	0.073%
45	12.210	1549	1551	1557	rVB2	10063	16498	0.44%	0.038%

46	12.822	1647	1655	1657	rBV9	7045	14999	0.40%	0.035%
47	12.910	1665	1670	1677	rVB2	11810	18332	0.49%	0.042%
48	13.298	1731	1736	1742	rVB7	9530	14433	0.38%	0.033%
49	13.369	1742	1748	1756	rBV4	24639	54952	1.46%	0.127%
50	13.881	1827	1835	1844	rBV	910768	1234373	32.85%	2.849%

51	14.157	1875	1882	1893	rBV	946957	1414944	37.66%	3.266%
52	14.469	1927	1935	1944	rBV	1372979	2069721	55.08%	4.778%
53	14.669	1962	1969	1980	rBV	279440	467310	12.44%	1.079%
54	14.822	1989	1995	2001	rBV	74660	111236	2.96%	0.257%
55	14.886	2003	2006	2012	rVV8	17103	27674	0.74%	0.064%

56	15.016	2024	2028	2032	rBV7	6015	8907	0.24%	0.021%
57	15.457	2096	2103	2112	rBV	1347948	1919280	51.08%	4.430%
58	15.575	2117	2123	2132	rVV	267804	378661	10.08%	0.874%
59	15.704	2141	2145	2150	rVB8	6856	11063	0.29%	0.026%
60	16.616	2297	2300	2306	rBV8	5667	9260	0.25%	0.021%

61	16.680	2306	2311	2317	rVV2	11158	22780	0.61%	0.053%
62	16.763	2320	2325	2331	rVB4	19981	31050	0.83%	0.072%
63	17.092	2377	2381	2384	rVB4	9031	12028	0.32%	0.028%
64	17.216	2390	2402	2412	rBV	1894663	2707908	72.07%	6.251%
65	17.316	2412	2419	2428	rVV	1376688	1998681	53.19%	4.614%

66	17.716	2483	2487	2492	rBV2	22451	28756	0.77%	0.066%
67	17.886	2514	2516	2521	rVB6	6704	9580	0.25%	0.022%
68	17.980	2528	2532	2537	rBV	27774	38298	1.02%	0.088%
69	18.104	2548	2553	2562	rBV	178835	258681	6.88%	0.597%
70	18.433	2605	2609	2612	rVB5	9805	14307	0.38%	0.033%

71	18.574	2629	2633	2637	rVB5	14062	17674	0.47%	0.041%
72	18.622	2638	2641	2644	rBV4	15499	21747	0.58%	0.050%
73	18.663	2644	2648	2653	rVB	111538	144081	3.83%	0.333%
74	18.880	2680	2685	2689	rBV	139632	173212	4.61%	0.400%
75	18.922	2689	2692	2696	rVB	42310	49132	1.31%	0.113%

76	19.004	2703	2706	2709	rBV5	19504	29581	0.79%	0.068%
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77	19.116	2720	2725	2726	rBV2	94377	142500	3.79%	0.329%
78	19.257	2745	2749	2754	rVB2	78286	101151	2.69%	0.233%
79	19.339	2759	2763	2769	rBV3	93860	122162	3.25%	0.282%
80	19.486	2784	2788	2792	rVB	206987	223652	5.95%	0.516%
81	19.551	2793	2799	2804	rVV	2139481	2820620	75.07%	6.511%
82	19.598	2804	2807	2812	rVB3	40318	47872	1.27%	0.111%
83	19.716	2825	2827	2833	rBV2	17144	24190	0.64%	0.056%
84	19.851	2847	2850	2852	rBV2	25161	29134	0.78%	0.067%
85	19.886	2853	2856	2860	rVB	27934	33949	0.90%	0.078%
86	20.080	2886	2889	2894	rVB	92185	101091	2.69%	0.233%
87	20.304	2924	2927	2931	rVB2	38306	38622	1.03%	0.089%
88	20.504	2957	2961	2965	rBV	154954	162949	4.34%	0.376%
89	20.563	2969	2971	2975	rVB3	51330	54010	1.44%	0.125%
90	20.727	2995	2999	3003	rBV2	201261	263326	7.01%	0.608%
91	20.910	3026	3030	3035	rBV	503117	588611	15.66%	1.359%
92	21.021	3045	3049	3051	rBV2	248881	328017	8.73%	0.757%
93	21.051	3051	3054	3058	rVB	641742	728515	19.39%	1.682%
94	21.298	3092	3096	3103	rVB	2612713	3396448	90.39%	7.840%
95	21.904	3196	3199	3202	rBV	172821	227835	6.06%	0.526%
96	22.945	3371	3376	3381	rVB	329929	510715	13.59%	1.179%
97	23.510	3465	3472	3478	rBV	1471625	2726219	72.55%	6.293%
98	23.662	3491	3498	3513	rVB	1761032	3568806	94.98%	8.238%
99	24.274	3598	3602	3611	rVB2	189669	374995	9.98%	0.866%
100	28.033	4231	4241	4258	rVB3	1035895	3757493	100.00%	8.674%

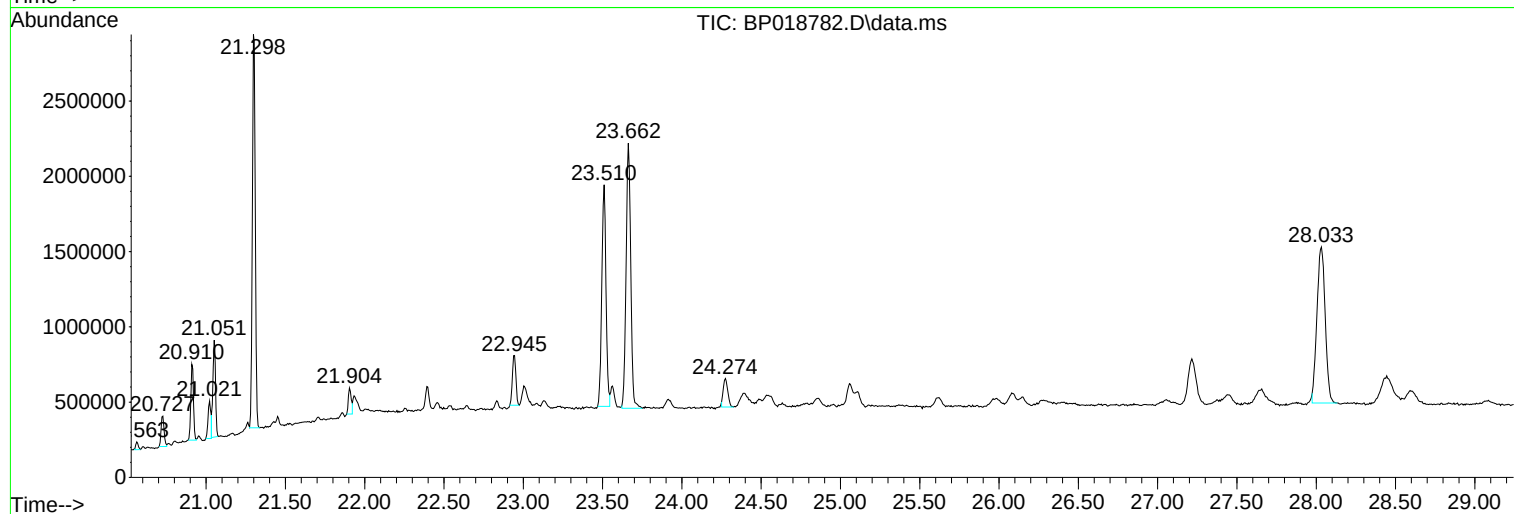
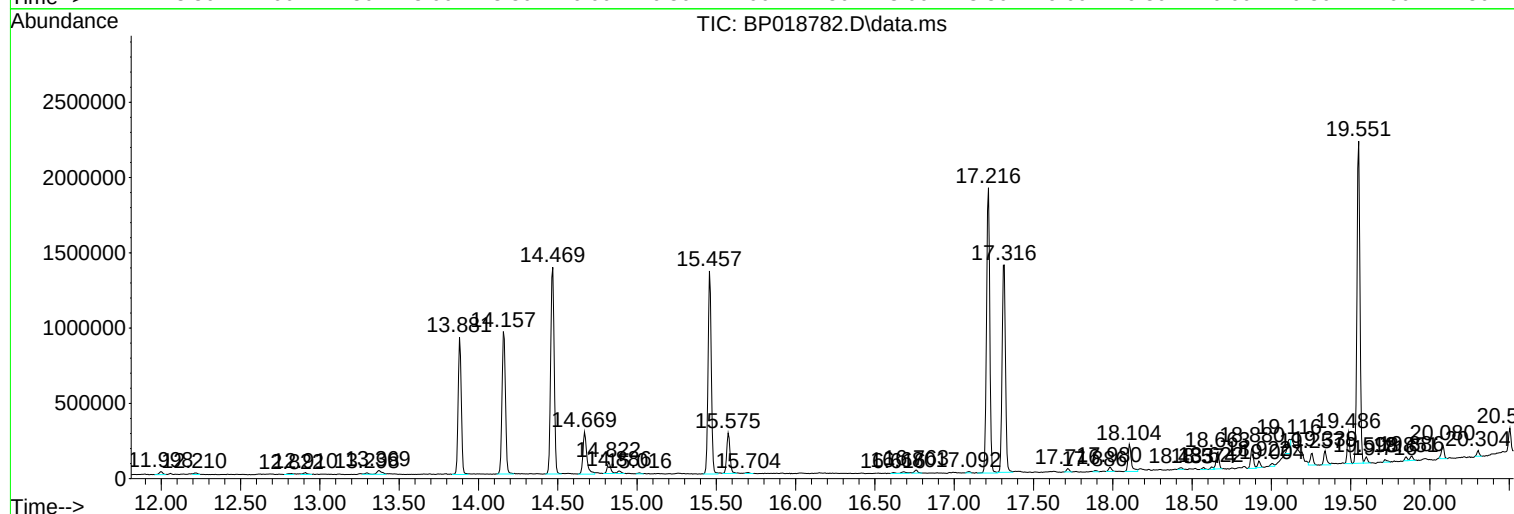
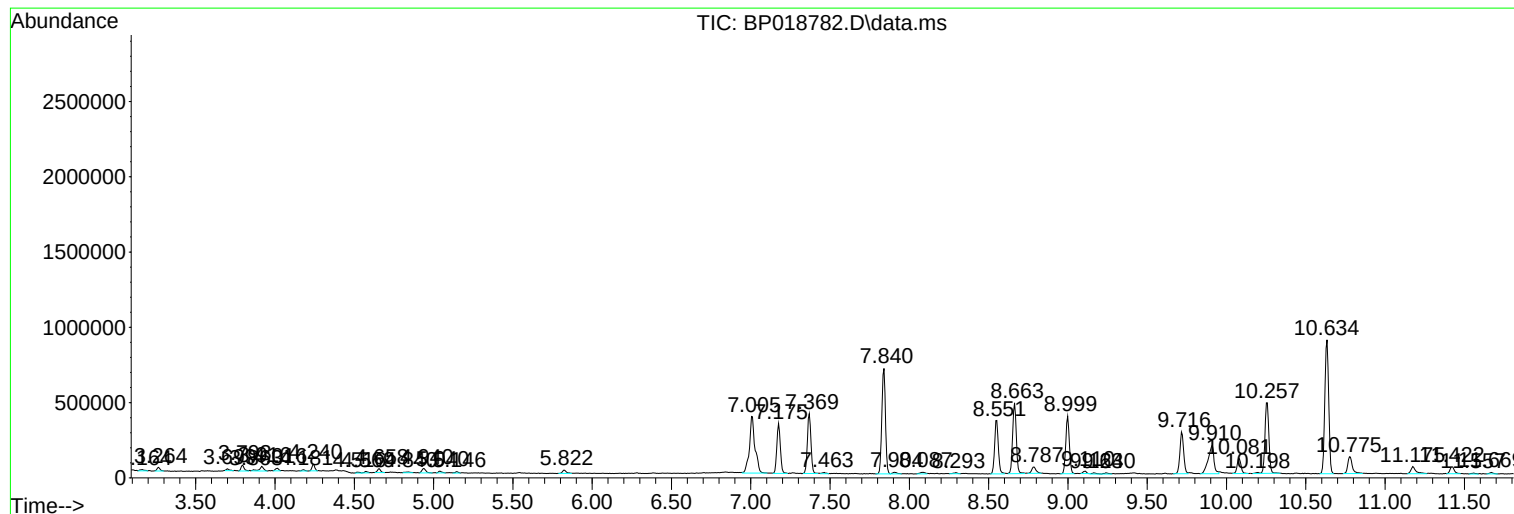
Sum of corrected areas: 43320762

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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



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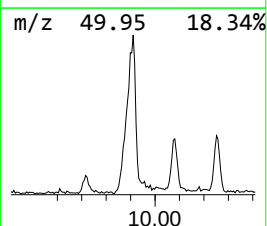
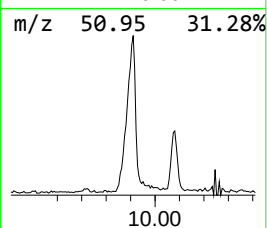
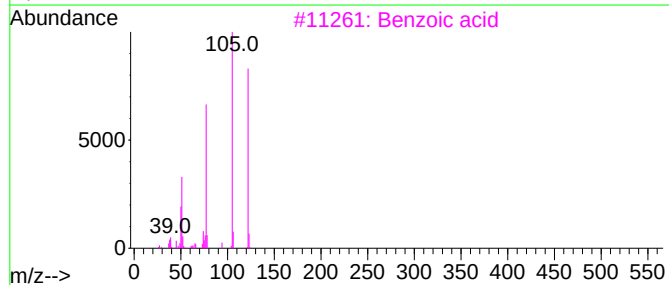
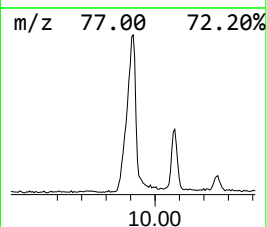
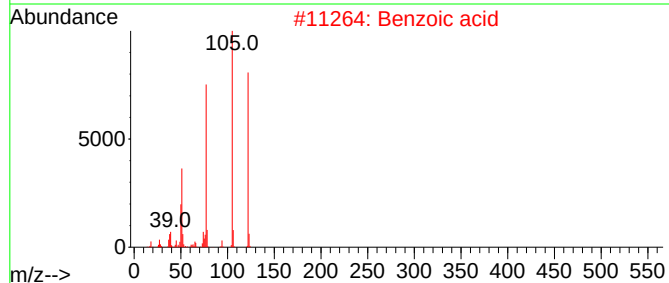
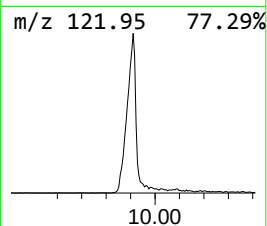
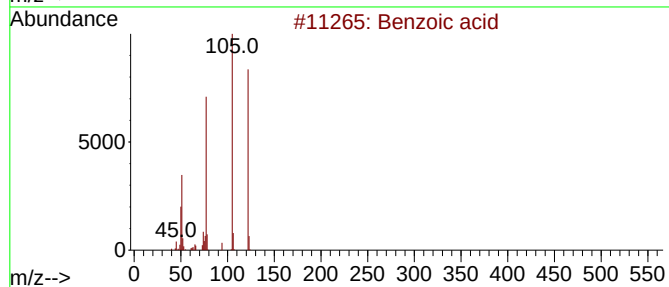
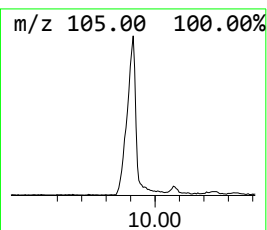
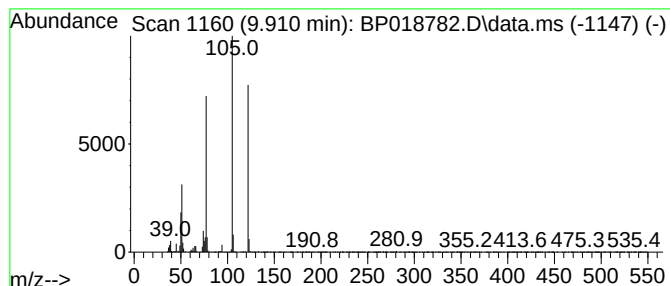
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.910	6.37 ng/ul	475241	Naphthalene-d8	10.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid	122	C7H6O2	000065-85-0	96
2			Benzoic acid	122	C7H6O2	000065-85-0	94
3			Benzoic acid	122	C7H6O2	000065-85-0	94
4			Benzoic acid, silver(1+) salt	228	C7H5AgO2	000532-31-0	90
5			2-Chloroethyl benzoate	184	C9H9ClO2	000939-55-9	83



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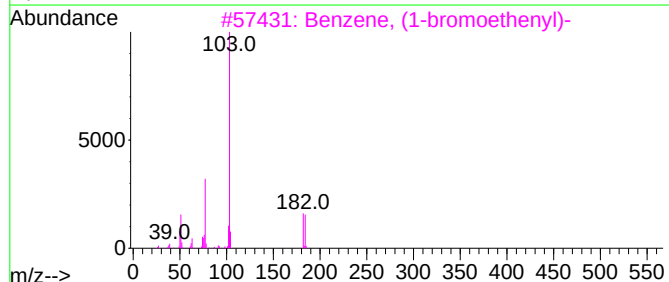
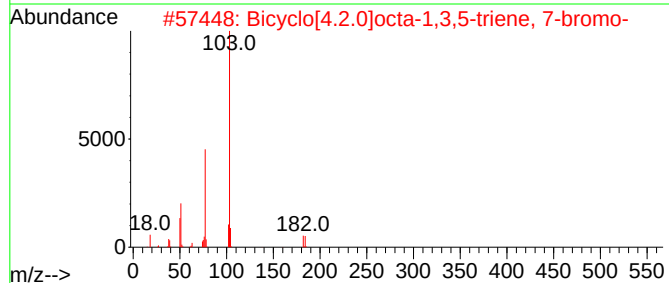
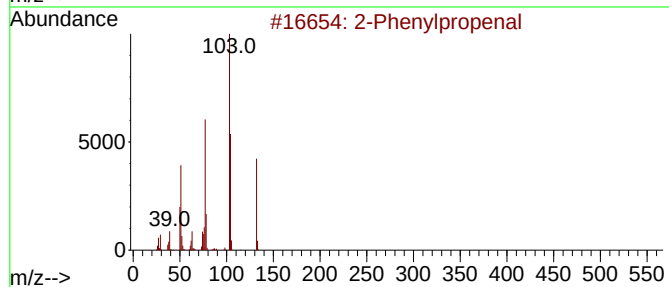
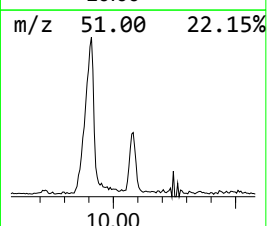
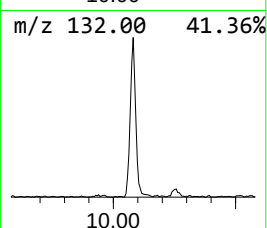
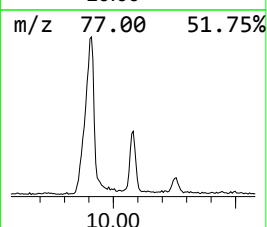
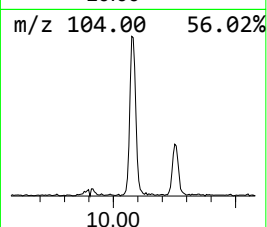
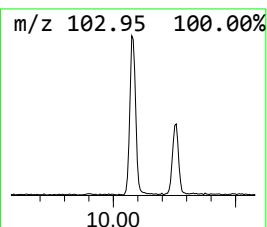
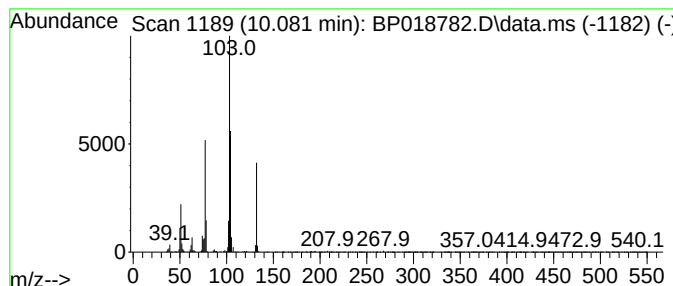
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 2-Phenylpropenal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.081	2.30 ng/ul	171345	Naphthalene-d8	10.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Phenylpropenal	132	C9H8O	004432-63-7	87
2			Bicyclo[4.2.0]octa-1,3,5-triene,...	182	C8H7Br	021120-91-2	50
3			Benzene, (1-bromoethenyl)-	182	C8H7Br	000098-81-7	47
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	182	C8H7Br	021120-91-2	47
5			5(4H)-Isoxazolone, 3-phenyl-	161	C9H7NO2	001076-59-1	45



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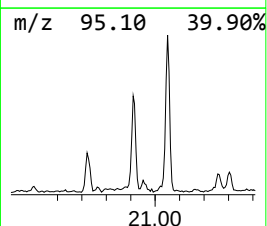
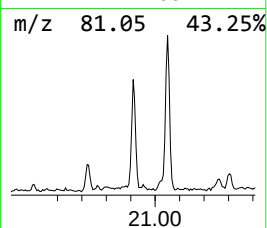
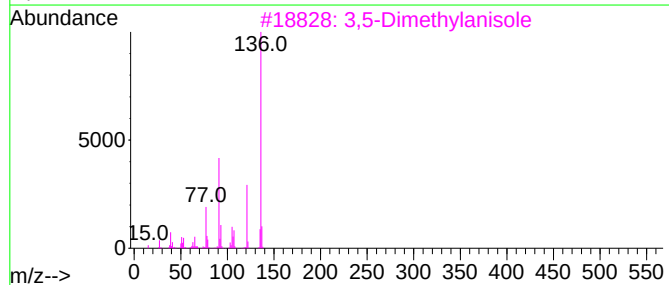
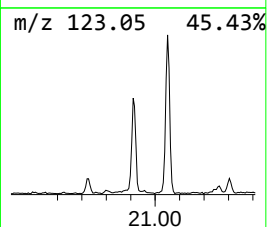
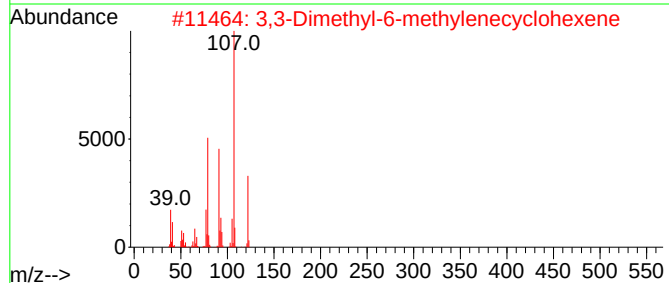
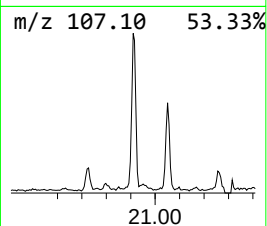
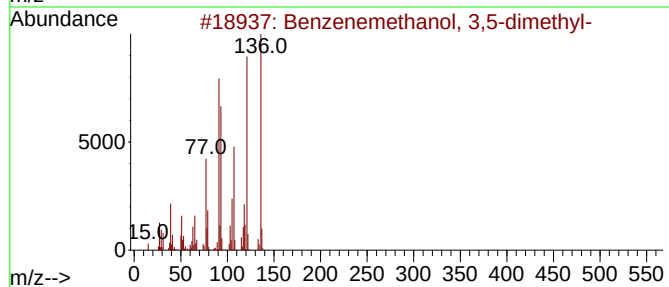
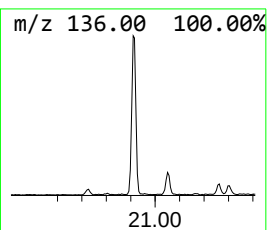
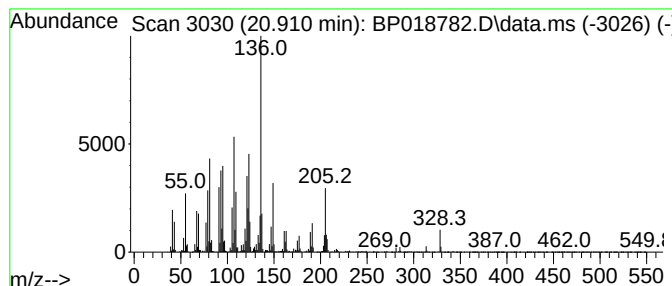
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.910	3.47 ng/ul	588611	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenemethanol, 3,5-dimethyl-	136	C9H12O	027129-87-9	27
2			3,3-Dimethyl-6-methylenecyclohexene	122	C9H14	020185-16-4	25
3			3,5-Dimethylanisole	136	C9H12O	000874-63-5	18
4			1-(Isocyanatomethyl)-4-propoxybe...	191	C11H13NO2	936095-07-7	15
5			Isobutyric acid, .alpha.-[2,4,5-...	222	C13H18O3	086550-00-7	14



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Data File : BP018782.D
Acq On : 12 Dec 2023 23:40
Operator : MA/JU
Sample : 05646-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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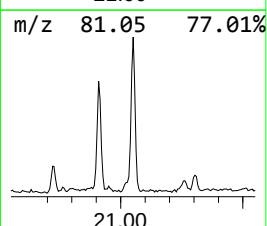
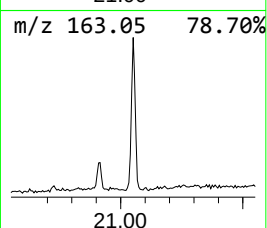
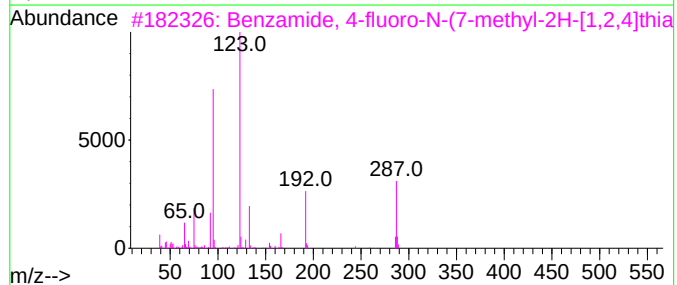
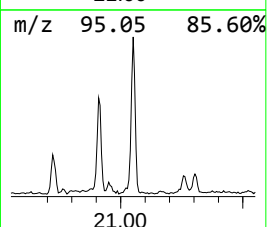
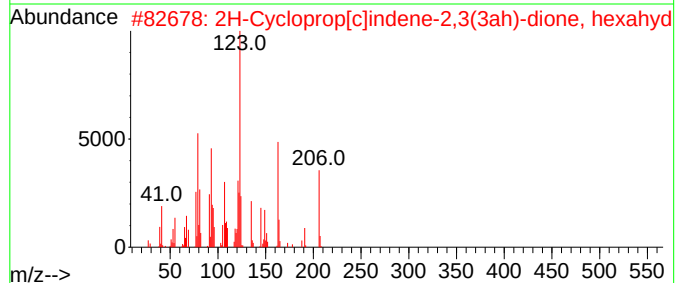
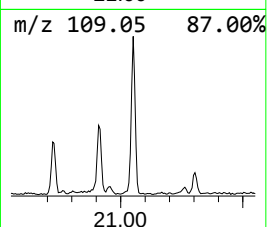
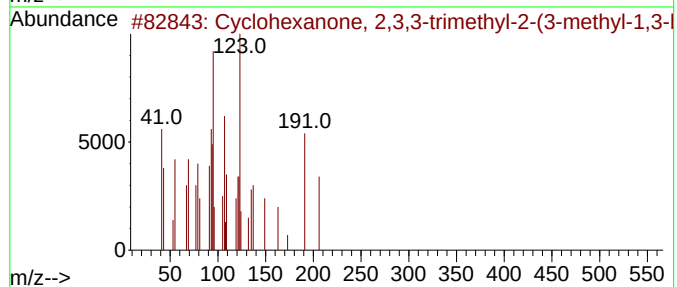
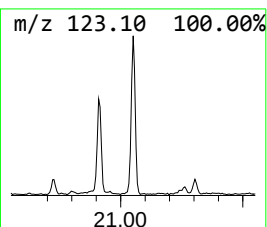
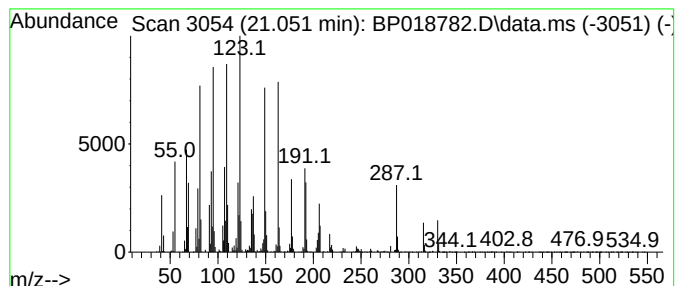
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	4.29 ng/ul	728515	Chrysene-d12	21.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	25
2			2H-Cycloprop[c]indene-2,3(3ah)-d...	206	C13H18O2	096678-99-8	25
3			Benzamide, 4-fluoro-N-(7-methyl-...	287	C14H10FN3OS	1000350-88-7	22
4			1-(2-Cyanoethyl)-2-ethyl-4-methy...	163	C9H13N3	023996-25-0	22
5			(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018782.D
Acq On : 12 Dec 2023 23:40
Operator : MA/JU
Sample : 05646-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

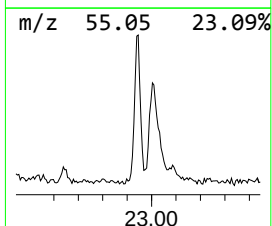
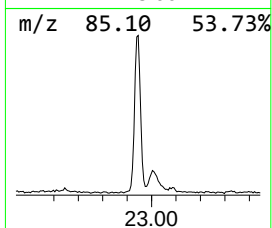
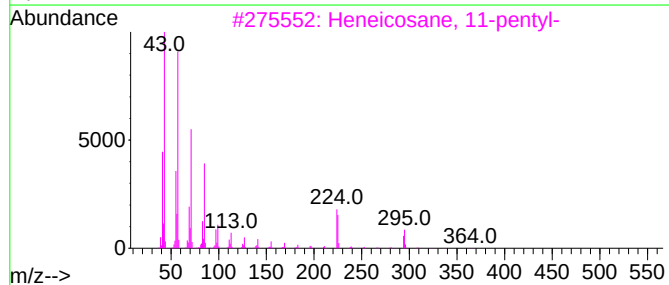
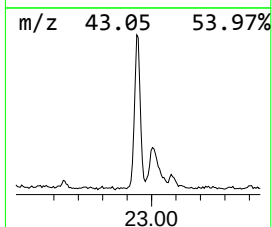
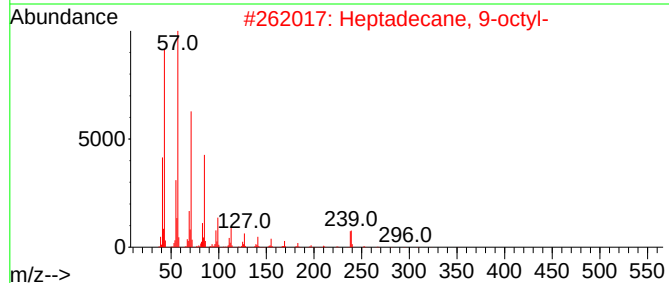
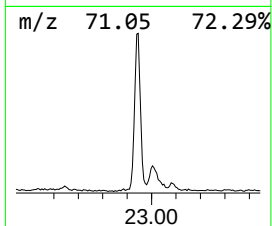
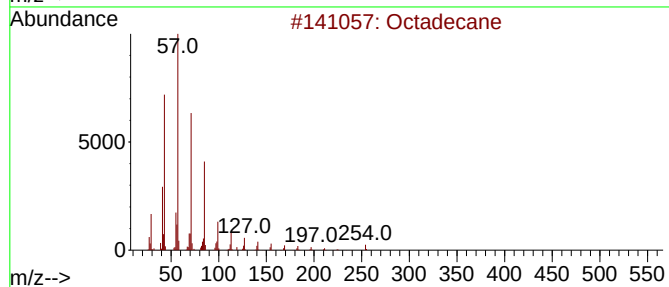
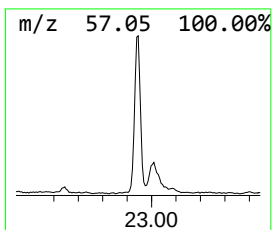
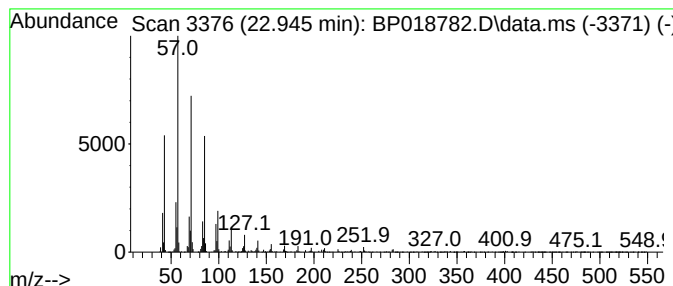
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.MA.M
Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.945	2.86 ng/ul	510715	Perylene-d12		23.663	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	95
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	93
3	Heneicosane, 11-pentyl-		366	C26H54	014739-72-1	91
4	Heneicosane		296	C21H44	000629-94-7	90
5	Triacontane		422	C30H62	000638-68-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018782.D
Acq On : 12 Dec 2023 23:40
Operator : MA/JU
Sample : 05646-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AY1

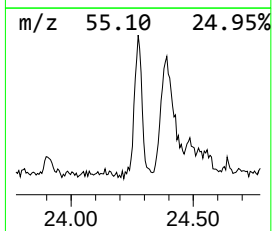
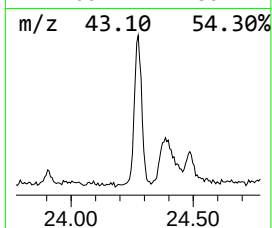
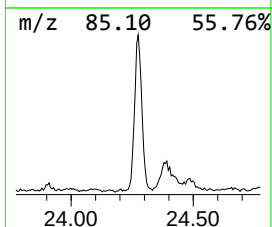
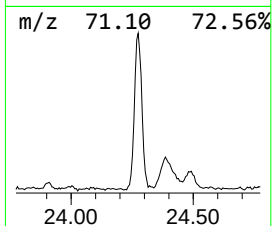
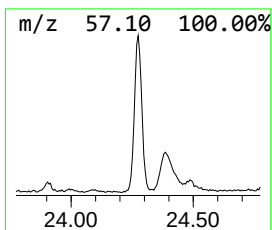
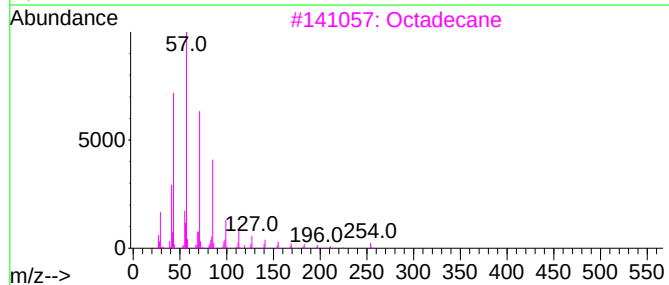
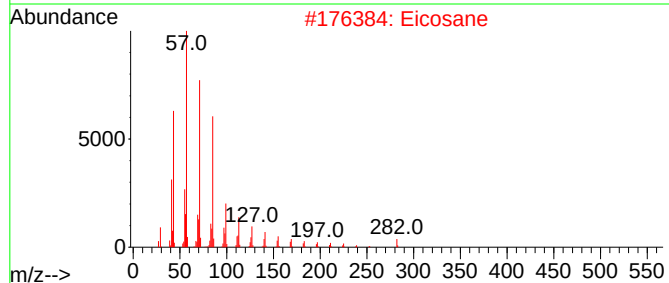
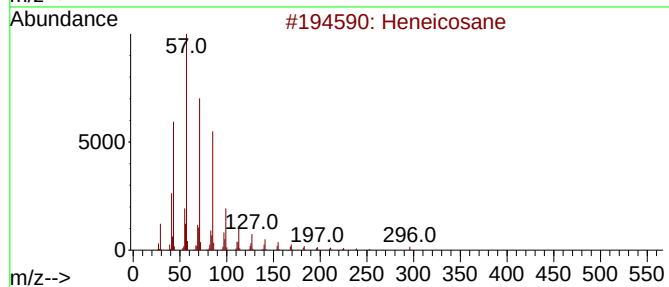
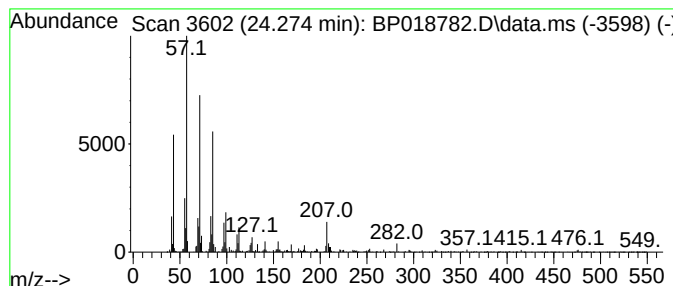
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.274	2.10 ng/ul	374995	Perylene-d12	23.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	96
2		Eicosane	282	C20H42	000112-95-8	95
3		Octadecane	254	C18H38	000593-45-3	95
4		Eicosane	282	C20H42	000112-95-8	91
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018782.D
Acq On : 12 Dec 2023 23:40
Operator : MA/JU
Sample : 05646-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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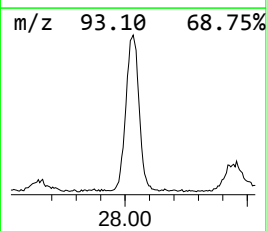
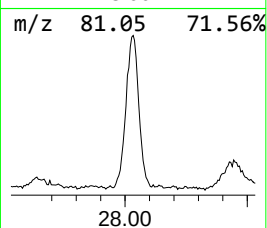
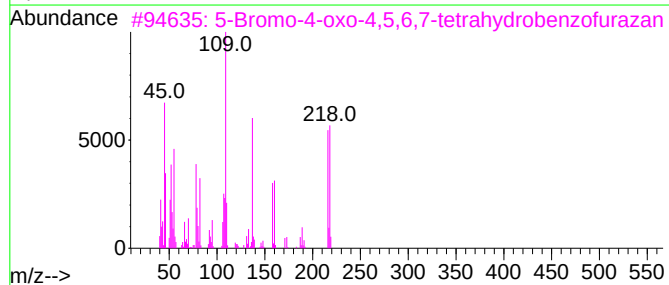
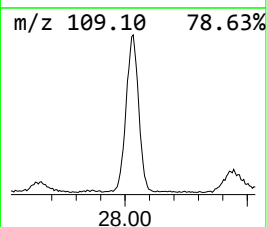
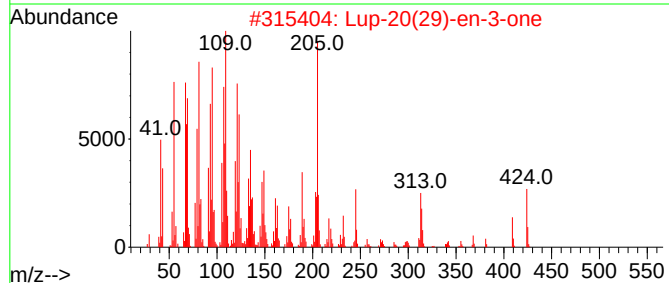
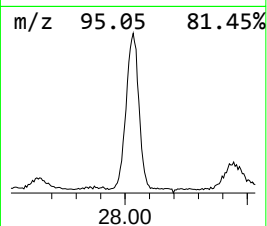
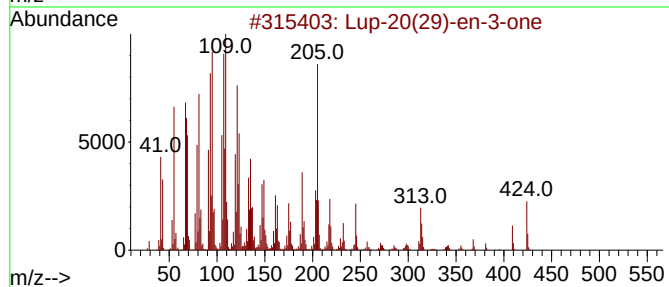
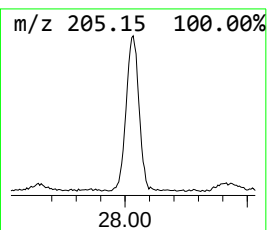
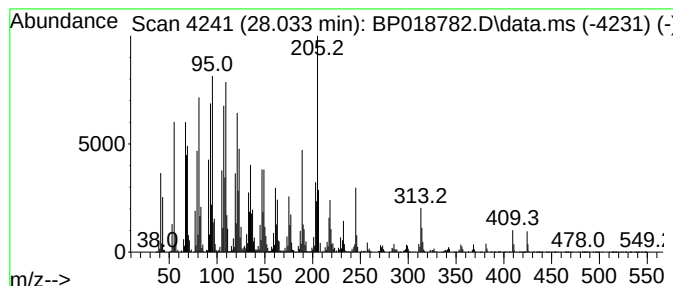
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Lup-20(29)-en-3-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.033	21.06 ng/ul	3757490	Perylene-d12	23.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
2			Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	99
3			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	91
4			Guaia-9,11-diene	204	C15H24	1000374-19-8	53
5			9,19-Cyclolanost-23-ene-3,25-dio...	442	C30H50O2	054482-57-4	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121123\
Data File : BP018782.D
Acq On : 12 Dec 2023 23:40
Operator : MA/JU
Sample : 05646-05
Misc :
ALS Vial : 61 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
C0AY1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120123.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	9.910	6.4	ng/ul	475241	2	10.634	1491440	20.0
2-Phenylpropenal	10.081	2.3	ng/ul	171345	2	10.634	1491440	20.0
unknown-01	20.910	3.5	ng/ul	588611	5	21.298	3396450	20.0
unknown-02	21.051	4.3	ng/ul	728515	5	21.298	3396450	20.0
(DEL) Alkane: S...	22.945	2.9	ng/ul	510715	6	23.663	3568810	20.0
(DEL) Alkane: S...	24.274	2.1	ng/ul	374995	6	23.663	3568810	20.0
Lup-20(29)-en-3...	28.033	21.1	ng/ul	3757490	6	23.663	3568810	20.0