

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
 Data File : BP010325.D
 Acq On : 12 May 2022 15:45
 Operator : CG/JU
 Sample : N2714-07
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 EW2X8

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-BP051022.M
 Title : SVOA CALIBRATION

Signal : TIC: BP010325.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	41	44	50	rBV2	19941	28752	0.69%	0.056%
2	3.775	115	117	129	rBV	76610	159989	3.85%	0.314%
3	4.093	167	171	177	rVB2	9399	14843	0.36%	0.029%
4	5.011	321	327	335	rBV2	29722	56953	1.37%	0.112%
5	6.428	565	568	573	rBV7	3620	7023	0.17%	0.014%
6	6.593	589	596	603	rVB3	14650	27212	0.65%	0.053%
7	6.899	642	648	654	rBV10	7847	13618	0.33%	0.027%
8	7.069	669	677	692	rBV	445614	777335	18.69%	1.526%
9	7.234	697	705	717	rVV	358895	619707	14.90%	1.216%
10	7.346	717	724	730	rVV3	51317	95922	2.31%	0.188%
11	7.434	732	739	753	rVV	469772	784876	18.87%	1.540%
12	7.534	753	756	763	rVB6	6446	10208	0.25%	0.020%
13	7.805	798	802	810	rVB2	26060	43719	1.05%	0.086%
14	7.905	812	819	827	rVV	508603	845127	20.32%	1.659%
15	7.975	827	831	838	rVB8	8759	16607	0.40%	0.033%
16	8.128	855	857	863	rBV7	3869	6428	0.15%	0.013%
17	8.187	863	867	874	rVB7	4516	8782	0.21%	0.017%
18	8.611	928	939	952	rBV	591599	1013813	24.37%	1.990%
19	8.734	955	960	965	rVB5	7001	14318	0.34%	0.028%
20	9.063	1008	1016	1026	rBV	470594	823983	19.81%	1.617%
21	9.234	1040	1045	1051	rVB9	4616	8630	0.21%	0.017%
22	9.505	1087	1091	1096	rBV5	6122	10475	0.25%	0.021%
23	9.787	1130	1139	1155	rBV	387819	687955	16.54%	1.350%
24	10.010	1171	1177	1183	rBV	3331	5751	0.14%	0.011%
25	10.116	1191	1195	1201	rVB6	11841	21097	0.51%	0.041%
26	10.328	1223	1231	1249	rBV	555627	1000143	24.04%	1.963%
27	10.481	1253	1257	1265	rVB4	10138	21665	0.52%	0.043%
28	10.705	1287	1295	1303	rBV	766840	1290758	31.03%	2.533%
29	10.840	1311	1318	1342	rBV	485192	975197	23.44%	1.914%
30	12.140	1535	1539	1544	rVB6	5945	8131	0.20%	0.016%
31	12.299	1560	1566	1574	rVB4	9479	20118	0.48%	0.039%
32	12.946	1673	1676	1683	rVB9	2756	4855	0.12%	0.010%
33	13.087	1694	1700	1703	rVB7	3030	5462	0.13%	0.011%
34	13.369	1742	1748	1753	rVB3	10334	15874	0.38%	0.031%
35	13.722	1804	1808	1811	rBV6	2283	4176	0.10%	0.008%
36	13.757	1811	1814	1821	rVB8	4511	7290	0.18%	0.014%

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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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37	13.863	1827	1832	1838	rBV9	2730	5536	0.13%	0.011%
38	13.940	1838	1845	1858	rBV	1161798	1738631	41.80%	3.412%
39	14.228	1886	1894	1908	rBV	1251026	1891910	45.48%	3.713%
40	14.440	1928	1930	1935	rVB6	4496	5105	0.12%	0.010%
41	14.534	1939	1946	1957	rBV	1296191	1870039	44.96%	3.670%
42	14.634	1960	1963	1967	rVB5	6620	8163	0.20%	0.016%
43	14.728	1971	1979	1997	rBV	359456	765656	18.41%	1.503%
44	14.957	2013	2018	2023	rVB7	11508	18955	0.46%	0.037%
45	15.345	2079	2084	2090	rBV7	5516	12454	0.30%	0.024%
46	15.528	2106	2115	2129	rBV	1747941	2516282	60.49%	4.939%
47	15.645	2129	2135	2151	rVV	526565	745798	17.93%	1.464%
48	15.763	2151	2155	2161	rVB	19368	30585	0.74%	0.060%
49	16.310	2246	2248	2253	rVB6	6885	8940	0.21%	0.018%
50	16.692	2309	2313	2316	rBV6	5548	7718	0.19%	0.015%
51	16.957	2354	2358	2359	rBV4	5300	6227	0.15%	0.012%
52	17.051	2370	2374	2376	rBV4	4134	5959	0.14%	0.012%
53	17.287	2406	2414	2424	rBV	1607488	2317857	55.72%	4.549%
54	17.387	2424	2431	2443	rVV2	1857789	2904561	69.83%	5.701%
55	17.481	2443	2447	2459	rVB2	20026	46280	1.11%	0.091%
56	17.663	2474	2478	2487	rBV10	6331	12378	0.30%	0.024%
57	17.957	2524	2528	2534	rVB2	23728	32312	0.78%	0.063%
58	18.057	2540	2545	2550	rBV5	23552	40890	0.98%	0.080%
59	18.169	2560	2564	2574	rBV	164706	278275	6.69%	0.546%
60	18.463	2611	2614	2616	rBV4	6472	7806	0.19%	0.015%
61	19.063	2714	2716	2721	rVB4	11243	15912	0.38%	0.031%
62	19.192	2734	2738	2745	rVB2	31592	48964	1.18%	0.096%
63	19.263	2746	2750	2753	rBV2	31473	45090	1.08%	0.088%
64	19.404	2770	2774	2780	rBV4	40394	69320	1.67%	0.136%
65	19.616	2804	2810	2816	rBV	2771941	3684471	88.57%	7.231%
66	20.139	2897	2899	2904	rVB2	50907	51257	1.23%	0.101%
67	20.622	2979	2981	2985	rVB	56831	54169	1.30%	0.106%
68	20.704	2991	2995	2998	rBV4	58923	72904	1.75%	0.143%
69	20.857	3006	3021	3030	rBV3	1127414	4159727	100.00%	8.164%
70	21.022	3047	3049	3054	rVB3	85646	109323	2.63%	0.215%
71	21.075	3054	3058	3067	rBV	666578	957528	23.02%	1.879%
72	21.245	3077	3087	3100	rVB2	1049385	3551209	85.37%	6.970%
73	21.369	3102	3108	3122	rVB	1785562	2489101	59.84%	4.885%
74	21.516	3131	3133	3137	rBV2	70002	80056	1.92%	0.157%
75	21.980	3208	3212	3225	rBV2	403283	745888	17.93%	1.464%
76	23.051	3389	3394	3399	rBV	550464	831861	20.00%	1.633%

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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

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Title : SVOA CALIBRATION

77	23.639	3487	3494	3500	rBV2	1819934	3522846	84.69%	6.914%
78	23.792	3513	3520	3534	rVB2	1287656	2812771	67.62%	5.521%
79	24.427	3623	3628	3636	rVB	233152	488245	11.74%	0.958%
80	24.521	3639	3644	3653	rVV3	158062	380533	9.15%	0.747%
81	28.727	4351	4359	4382	rVB6	485461	2044556	49.15%	4.013%

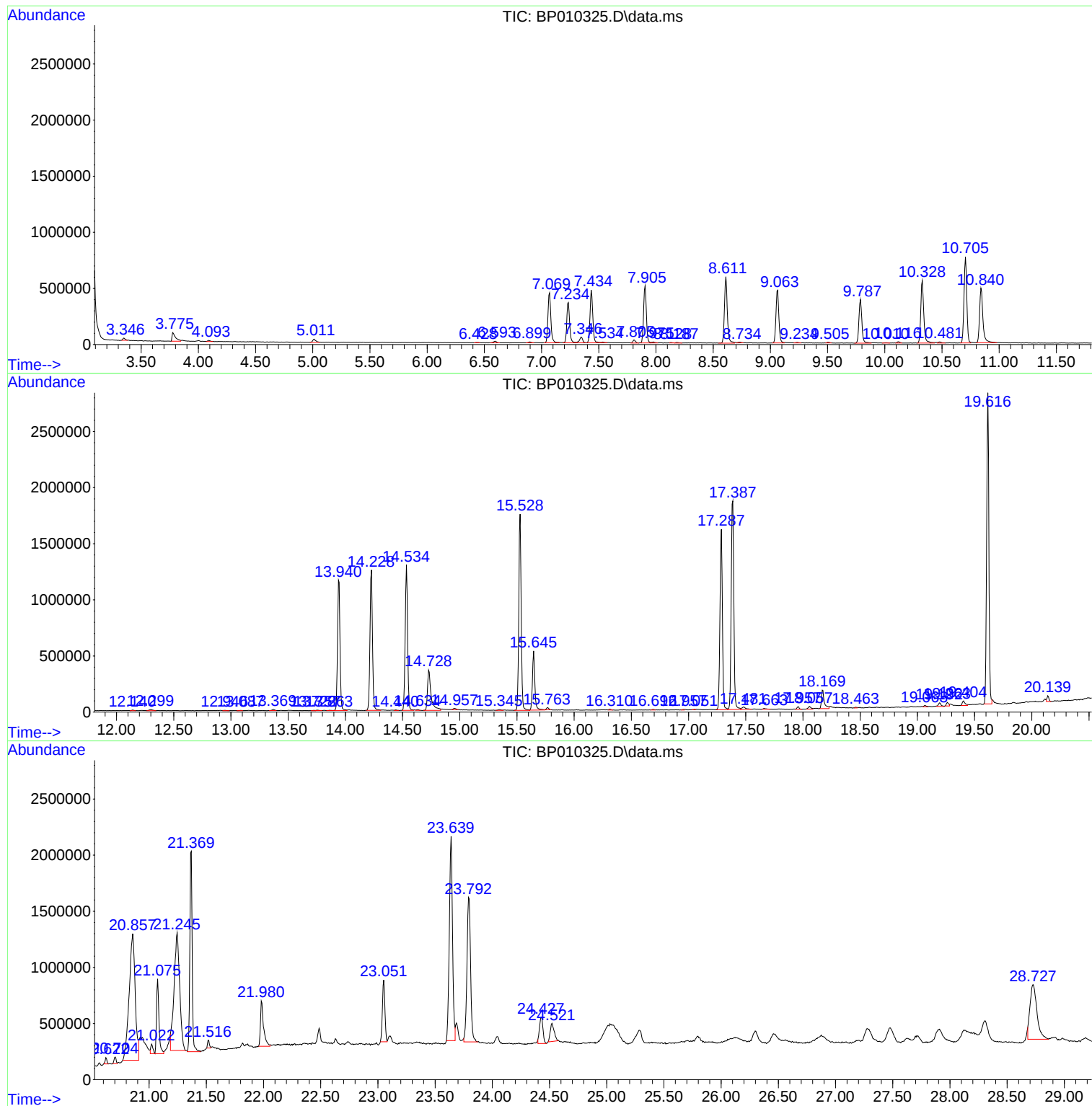
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Misc :
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Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051022.M
Quant Title : SVOA CALIBRATION

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



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Acq On : 12 May 2022 15:45
Operator : CG/JU
Sample : N2714-07
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EW2X8

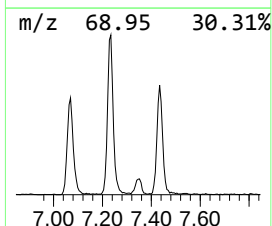
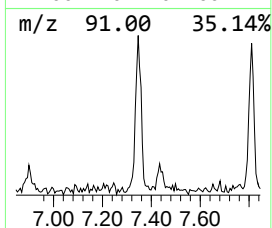
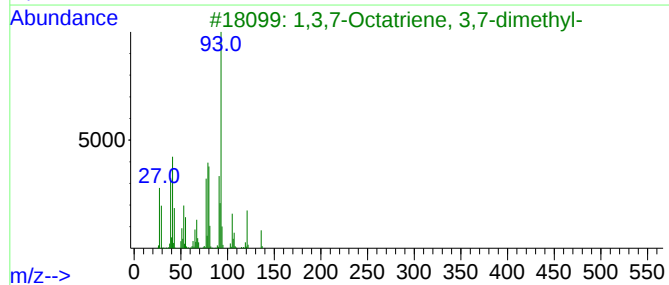
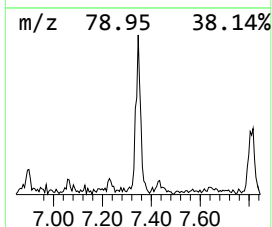
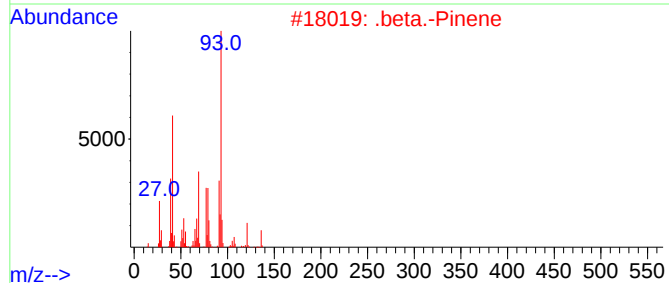
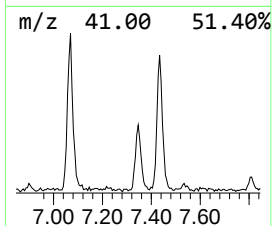
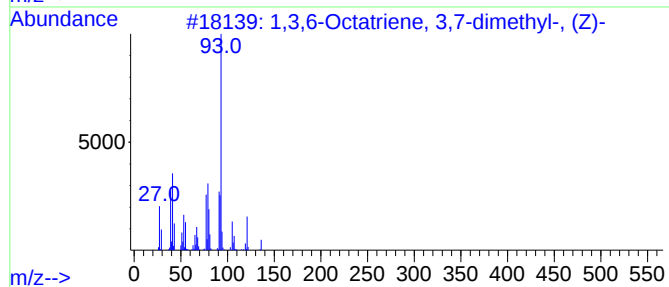
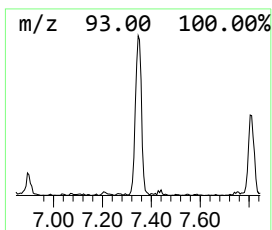
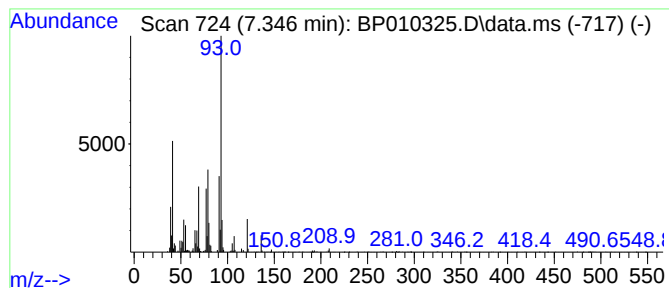
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051022.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,3,6-Octatriene, 3,7-dimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.346	2.27 ng/ul	95922	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	87		
2	.beta.-Pinene	136	C10H16	000127-91-3	87		
3	1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	87		
4	Cyclopropane, 1,1-dimethyl-2-(3-...	136	C10H16	068998-21-0	86		
5	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	86		



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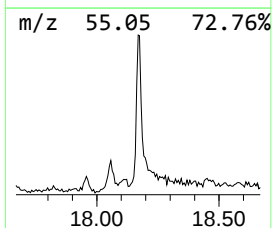
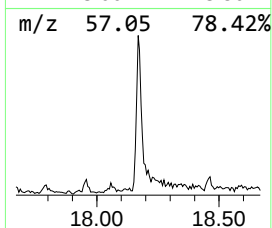
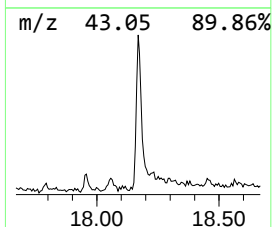
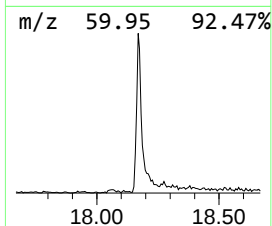
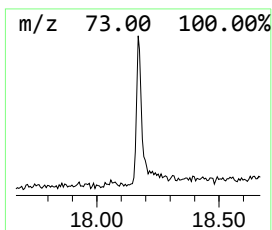
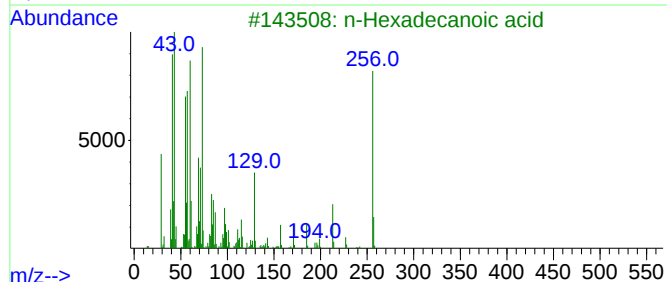
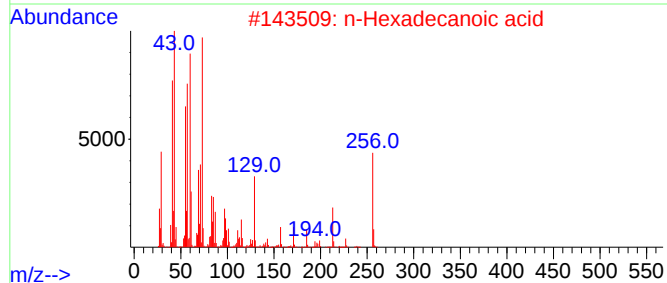
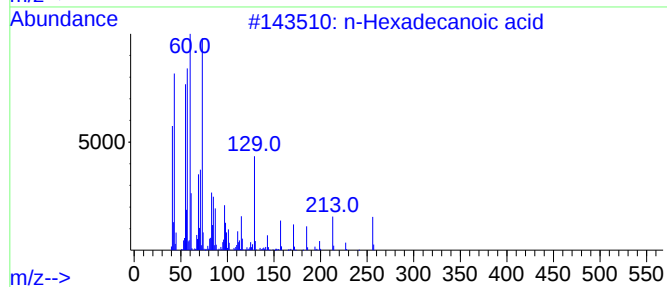
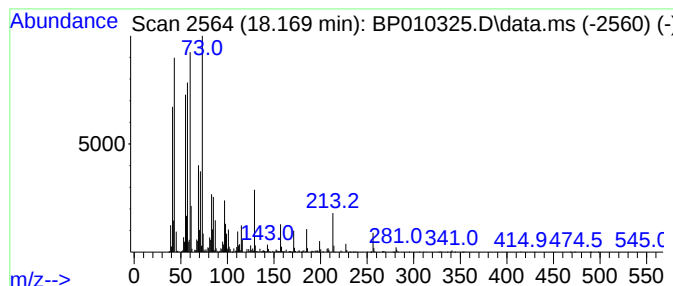
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051022.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.169	2.40 ng/ul	278275	Phenanthrene-d10	17.287

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	98
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93



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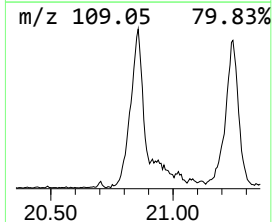
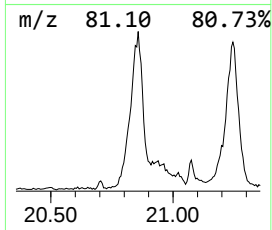
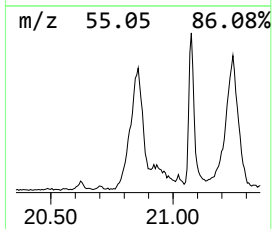
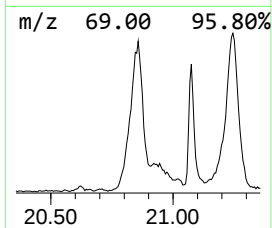
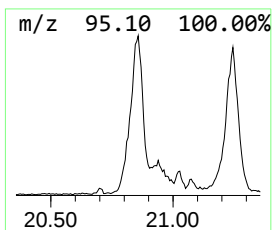
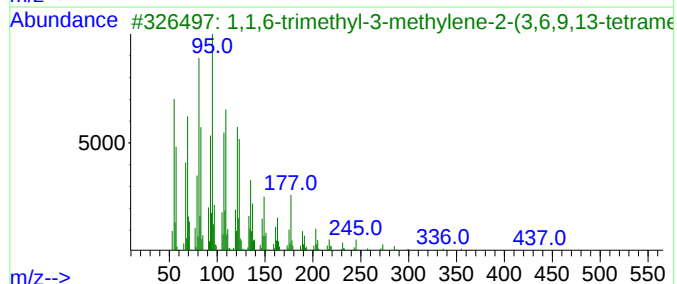
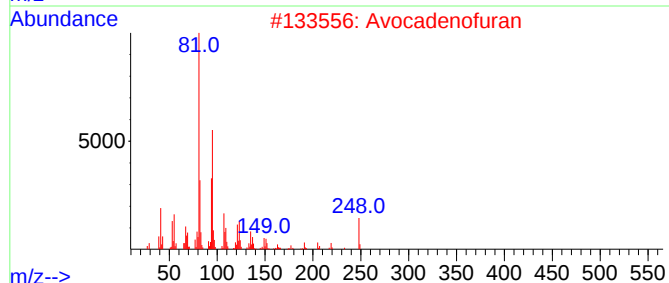
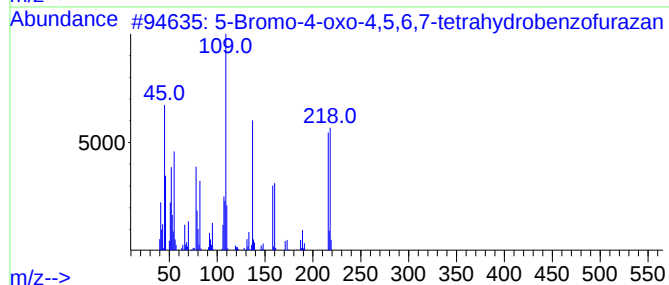
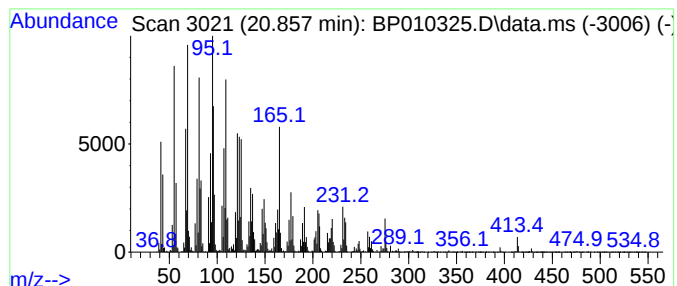
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.857	33.42 ng/ul	4159730	Chrysene-d12	21.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	90
2	Avocadenofuran	248	C17H28O	025346-24-1	87
3	1,1,6-trimethyl-3-methylene-2-(3...	452	C33H56	1000373-94-5	78
4	Corymbolone	236	C15H24O2	097094-19-4	64
5	2,2,4a,6a,8a,9,12b,14a-Octamethy...	410	C30H50	053013-35-7	56



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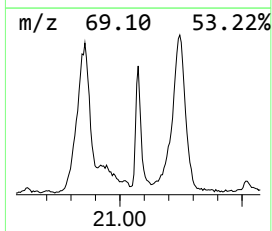
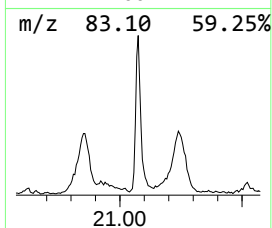
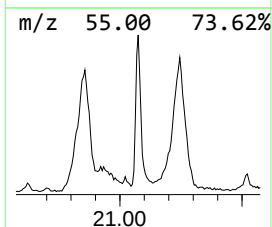
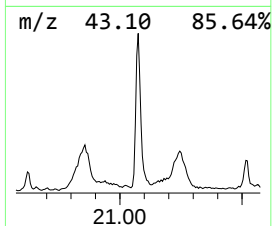
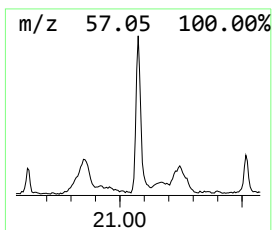
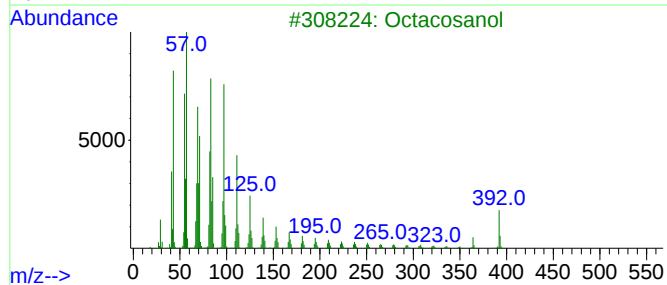
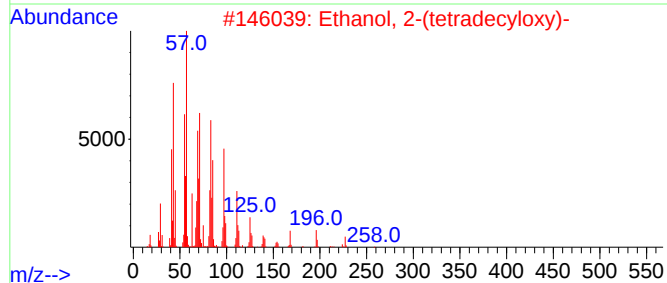
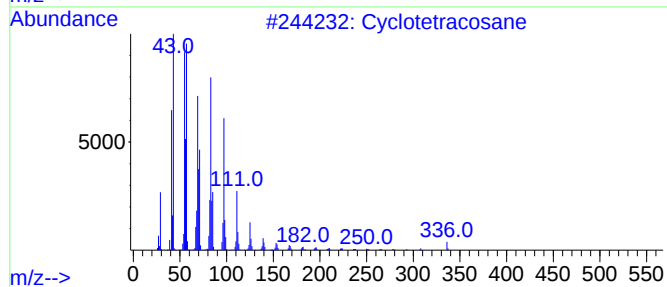
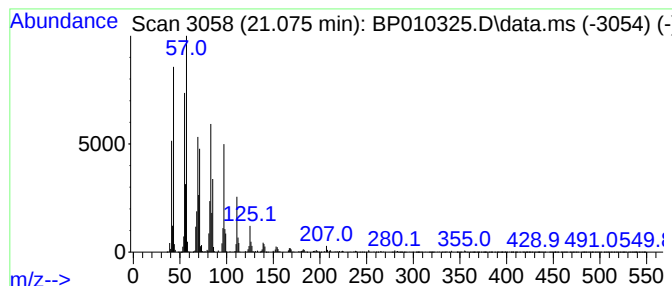
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051022.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Cyclic21.075 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.075	7.69 ng/ul	957528	Chrysene-d12	21.369	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	97
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	96
3	Octacosanol	410	C28H58O	000557-61-9	95
4	1-Octadecene	252	C18H36	000112-88-9	94
5	1-Hexacosene	364	C26H52	018835-33-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
Operator : CG/JU
Sample : N2714-07
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EW2X8

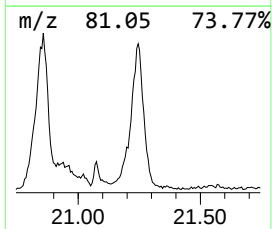
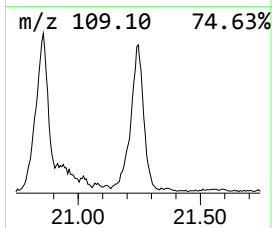
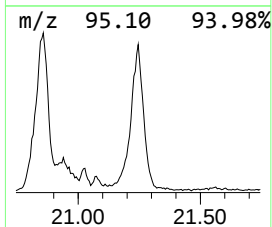
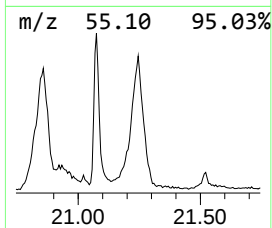
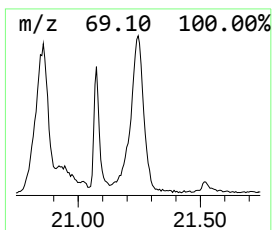
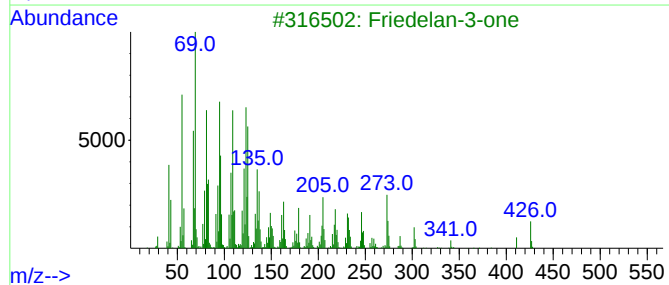
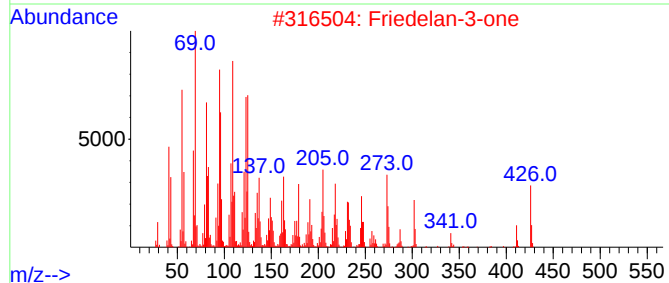
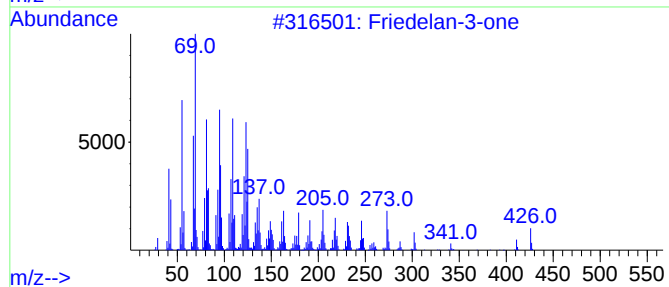
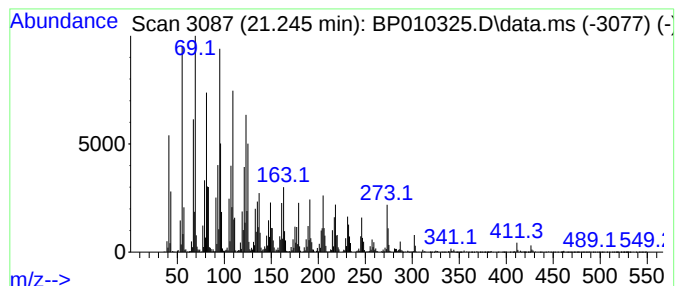
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Costunolide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.245	28.53 ng/ul	3551210	Chrysene-d12	21.369

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Friedelan-3-one	426	C30H50O	000559-74-0	99
2			Friedelan-3-one	426	C30H50O	000559-74-0	95
3			Friedelan-3-one	426	C30H50O	000559-74-0	90
4			Costunolide	232	C15H20O2	000553-21-9	64
5			Sesquirosefuran	218	C15H22O	039007-93-7	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
Operator : CG/JU
Sample : N2714-07
Misc :
ALS Vial : 49 Sample Multiplier: 1

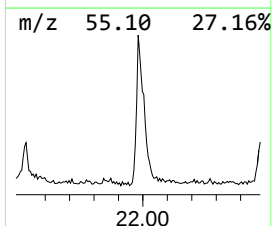
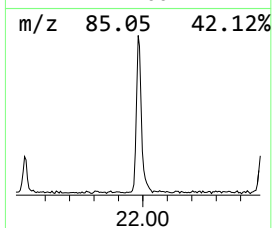
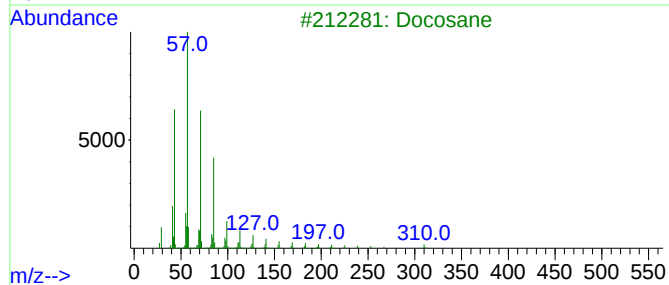
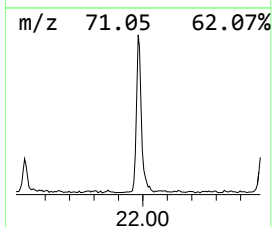
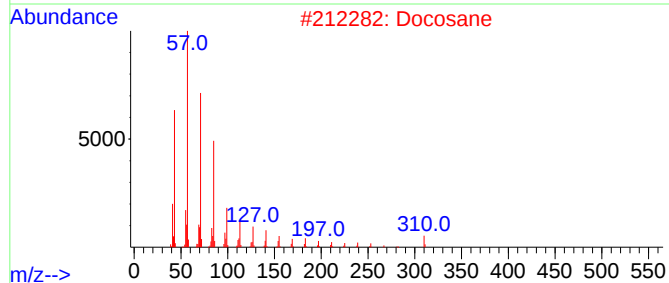
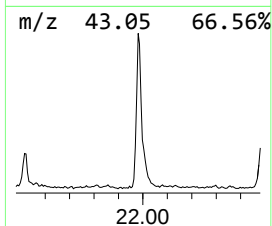
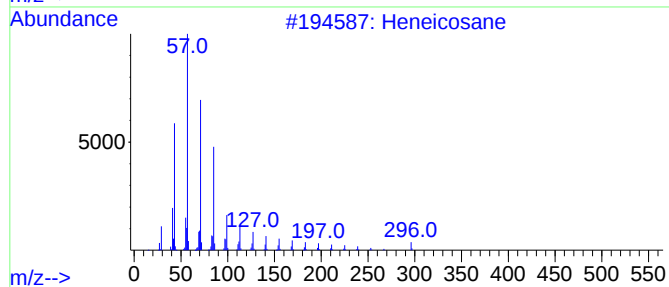
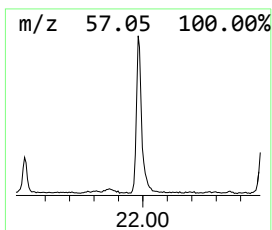
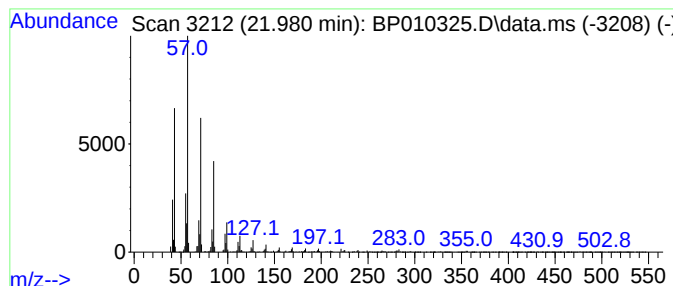
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.980	5.99 ng/ul	745888	Chrysene-d12		21.369	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Docosane		310	C22H46	000629-97-0	95
3	Docosane		310	C22H46	000629-97-0	94
4	Octadecane, 2-methyl-		268	C19H40	001560-88-9	93
5	Octacosane		394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
Operator : CG/JU
Sample : N2714-07
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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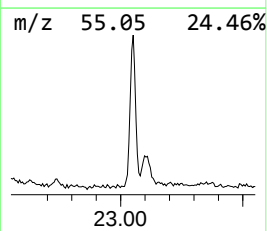
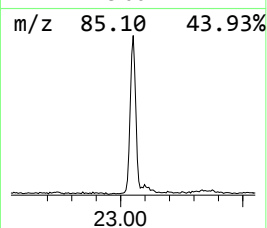
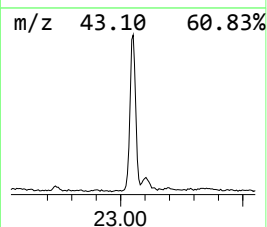
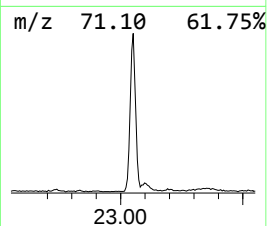
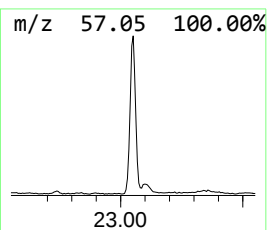
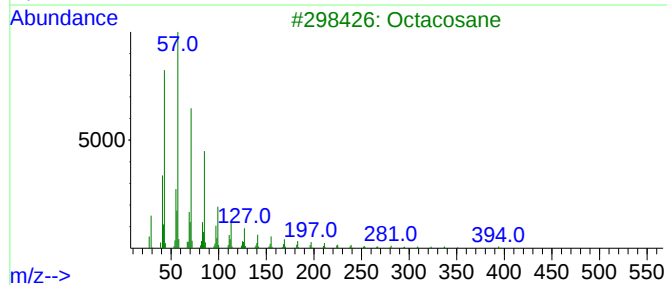
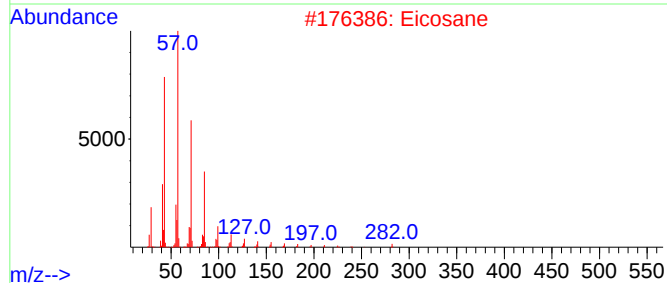
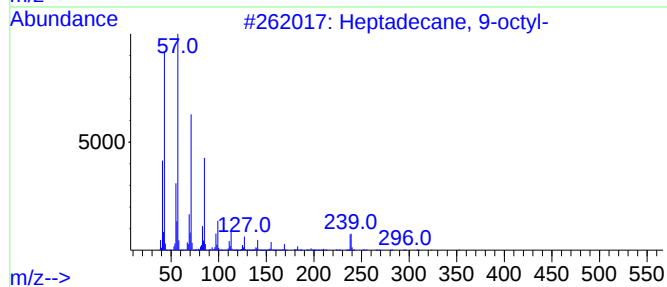
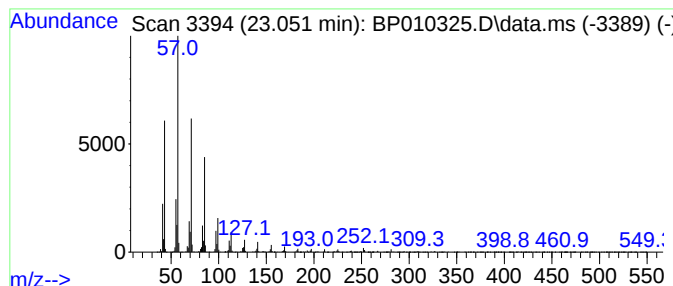
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.051	5.91 ng/ul	831861	Perylene-d12	23.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	96
2			Eicosane	282	C20H42	000112-95-8	95
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
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Sample : N2714-07
Misc :
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Instrument :
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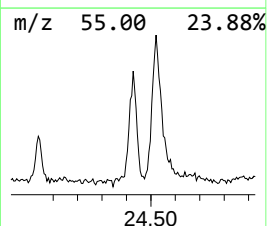
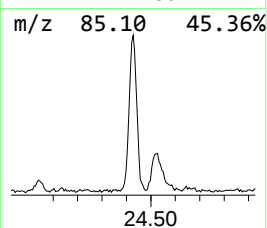
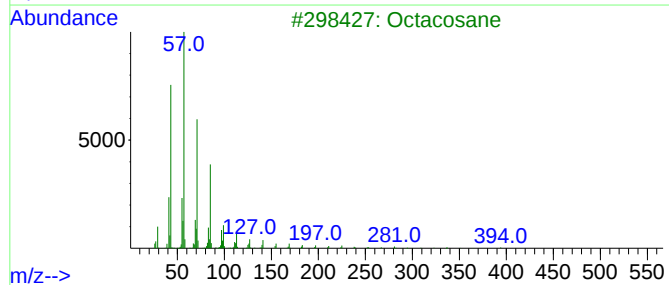
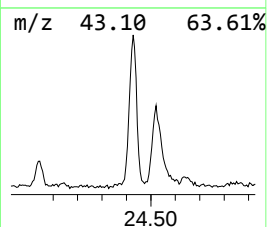
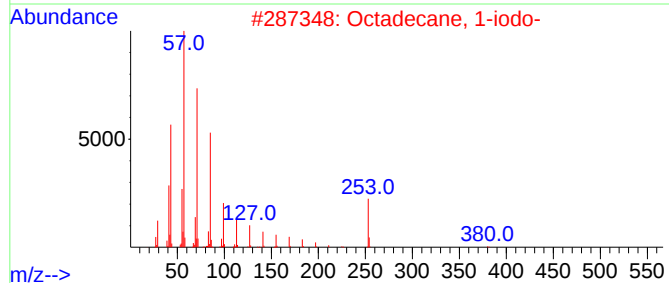
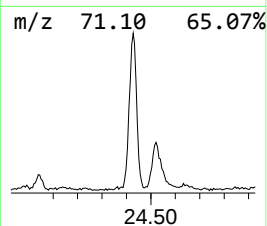
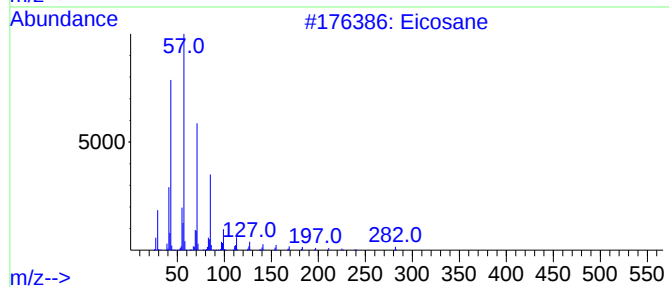
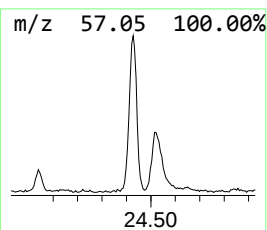
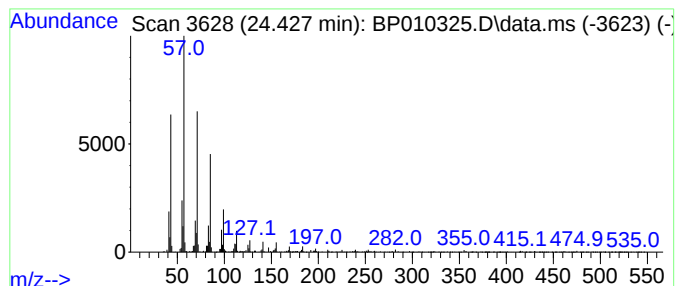
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.427	3.47 ng/ul	488245	Perylene-d12	23.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	92
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	91
3			Octacosane	394	C28H58	000630-02-4	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
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Sample : N2714-07
Misc :
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ClientSampleId :
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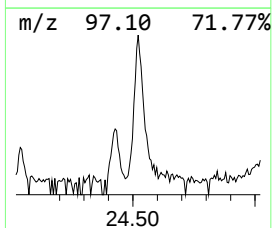
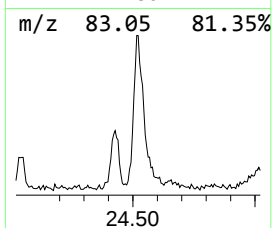
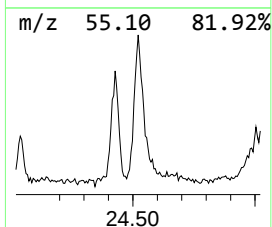
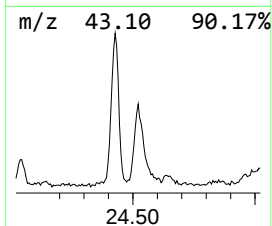
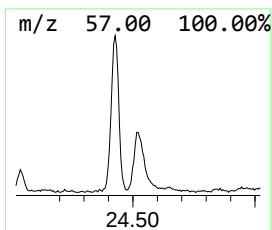
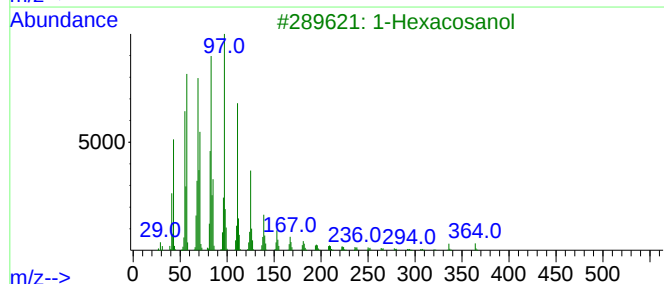
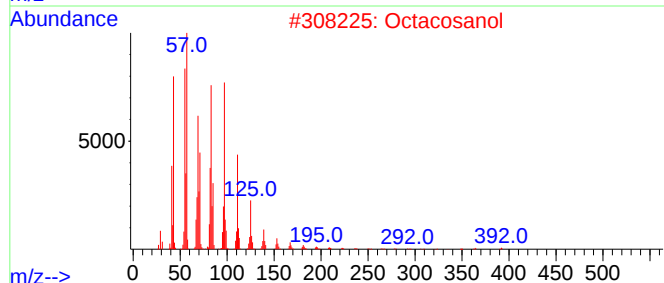
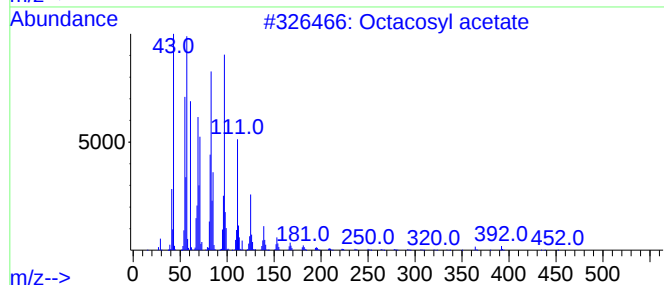
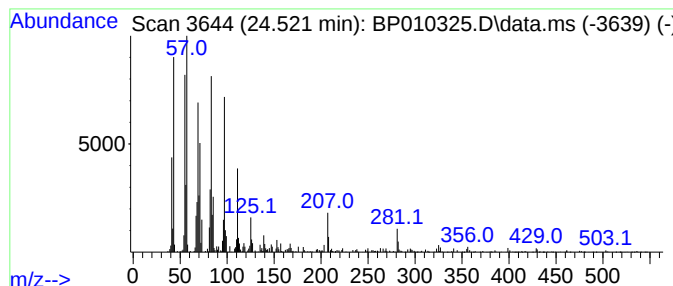
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Octacosyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.522	2.71 ng/ul	380533	Perylene-d12	23.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl acetate	452	C30H60O2	018206-97-8	92
2			Octacosanol	410	C28H58O	000557-61-9	91
3			1-Hexacosanol	382	C26H54O	000506-52-5	90
4			1-Heptacosanol	396	C27H56O	002004-39-9	90
5			Ethyl triacontyl ether	467	C32H66O	1000406-37-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
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ALS Vial : 49 Sample Multiplier: 1

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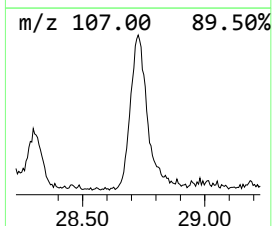
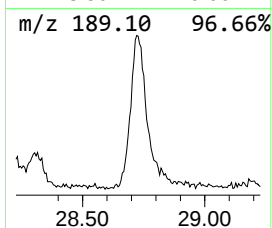
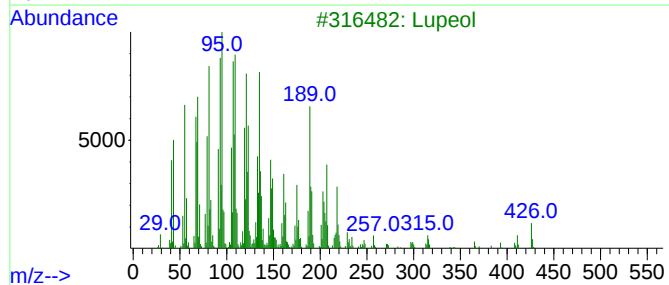
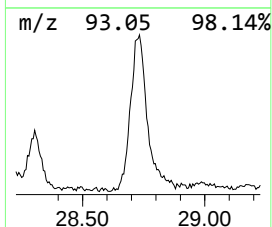
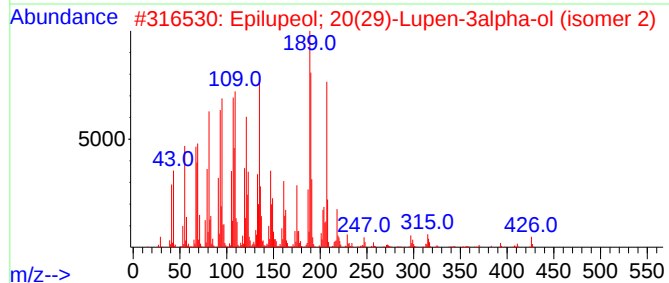
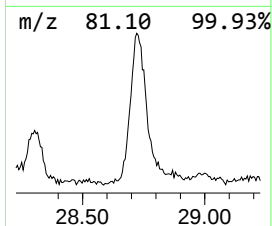
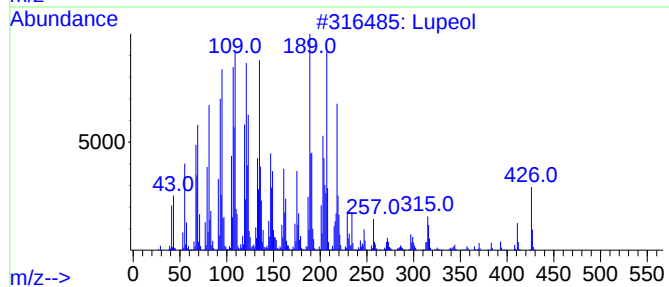
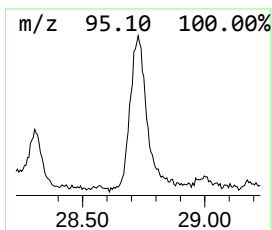
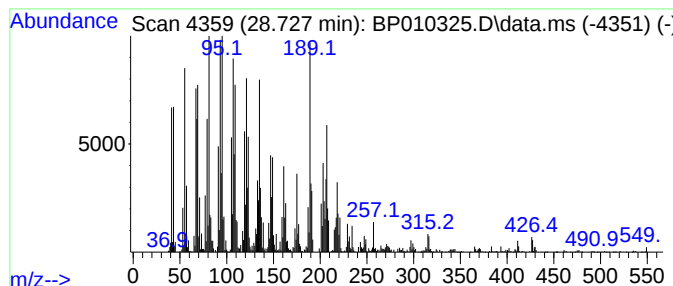
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 Lupeol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.727	14.54 ng/ul	2044560	Perylene-d12	23.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lupeol	426	C30H50O	000545-47-1	99
2			Epilupeol; 20(29)-Lupen-3alpha-o...	426	C30H50O	1000513-01-4	94
3			Lupeol	426	C30H50O	000545-47-1	90
4			Lup-20(29)-en-3-ol, acetate, (3...	468	C32H52O2	001617-68-1	90
5			Lupeol	426	C30H50O	000545-47-1	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051122\
Data File : BP010325.D
Acq On : 12 May 2022 15:45
Operator : CG/JU
Sample : N2714-07
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
EW2X8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP051022.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
1,3,6-Octatrien...	7.346	2.3	ng/ul	95922	1	7.905	845127	20.0
n-Hexadecanoic ...	18.169	2.4	ng/ul	278275	4	17.287	2317860	20.0
5-Bromo-4-oxo-4...	20.857	33.4	ng/ul	4159730	5	21.369	2489100	20.0
(DEL) Alkane: C...	21.075	7.7	ng/ul	957528	5	21.369	2489100	20.0
Costunolide	21.245	28.5	ng/ul	3551210	5	21.369	2489100	20.0
(DEL) Alkane: S...	21.980	6.0	ng/ul	745888	5	21.369	2489100	20.0
(DEL) Alkane: S...	23.051	5.9	ng/ul	831861	6	23.792	2812770	20.0
(DEL) Alkane: S...	24.427	3.5	ng/ul	488245	6	23.792	2812770	20.0
Octacosyl acetate	24.522	2.7	ng/ul	380533	6	23.792	2812770	20.0
Lupeol	28.727	14.5	ng/ul	2044560	6	23.792	2812770	20.0