

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
 Data File : BN024899.D
 Acq On : 14 Apr 2023 15:54
 Operator : CG/JU
 Sample : 02252-07
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 COME3

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_N\Methods\SFAM-EPA-BN041023.M
 Title : SVOA CALIBRATION

Signal : TIC: BN024899.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.311	17	21	32	rVB	71213	110984	0.95%	0.096%
2	3.746	94	95	111	rBV	177128	307474	2.64%	0.265%
3	3.975	128	134	140	rVB5	8787	17418	0.15%	0.015%
4	4.070	146	150	155	rBV	28592	41882	0.36%	0.036%
5	5.011	305	310	317	rVB6	7211	13942	0.12%	0.012%
6	5.222	339	346	360	rVB	240934	387312	3.33%	0.334%
7	7.099	658	665	676	rVB	332970	530516	4.56%	0.457%
8	7.269	687	694	698	rBV	1244760	1993423	17.13%	1.717%
9	7.464	721	727	738	rBV	1178172	1903006	16.36%	1.640%
10	7.828	783	789	794	rVB6	8110	13506	0.12%	0.012%
11	7.940	801	808	812	rBV	1318558	2128357	18.29%	1.834%
12	7.975	812	814	821	rVB	232577	297008	2.55%	0.256%
13	8.293	862	868	877	rVB	114428	187632	1.61%	0.162%
14	8.493	899	902	908	rVB7	6800	12734	0.11%	0.011%
15	8.652	920	929	944	rBV	951657	1498958	12.88%	1.291%
16	9.110	999	1007	1018	rBV	1562326	2559386	22.00%	2.205%
17	9.216	1021	1025	1031	rVV3	13494	24663	0.21%	0.021%
18	9.275	1031	1035	1041	rVB7	8797	16132	0.14%	0.014%
19	9.516	1070	1076	1083	rVB2	10738	17914	0.15%	0.015%
20	9.834	1122	1130	1144	rBV	1247531	2040656	17.54%	1.758%
21	10.369	1214	1221	1230	rBV	1689863	2800137	24.07%	2.412%
22	10.616	1259	1263	1267	rBV6	7052	12522	0.11%	0.011%
23	10.652	1267	1269	1277	rVV7	6990	12417	0.11%	0.011%
24	10.752	1277	1286	1297	rVB	1860956	3060697	26.31%	2.637%
25	10.893	1303	1310	1318	rBV	358118	633899	5.45%	0.546%
26	11.140	1347	1352	1357	rVB7	7049	14138	0.12%	0.012%
27	11.275	1364	1375	1383	rVB2	66280	110851	0.95%	0.096%
28	11.540	1414	1420	1430	rBV5	15725	29781	0.26%	0.026%
29	12.134	1514	1521	1531	rBV	1299079	1970492	16.94%	1.698%
30	12.222	1532	1536	1539	rVV5	19695	30193	0.26%	0.026%
31	12.275	1539	1545	1549	rVV2	139880	215630	1.85%	0.186%
32	12.316	1549	1552	1553	rVV3	23823	30226	0.26%	0.026%
33	12.340	1553	1556	1561	rVV2	32412	51953	0.45%	0.045%
34	12.410	1564	1568	1573	rVB3	25755	39220	0.34%	0.034%
35	12.563	1589	1594	1597	rBV7	15035	26411	0.23%	0.023%
36	12.616	1597	1603	1610	rVV	1245090	1808163	15.54%	1.558%

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37	12.751	1621	1626	1628	rBV6	13816	20254	0.17%	0.017%
38	12.793	1630	1633	1642	rVV9	14795	46690	0.40%	0.040%
39	12.904	1645	1652	1661	rVB8	32442	90098	0.77%	0.078%
40	13.404	1733	1737	1744	rVB2	15980	23759	0.20%	0.020%
41	13.551	1755	1762	1766	rBV10	7462	13715	0.12%	0.012%
42	13.887	1812	1819	1824	rVB8	9828	19928	0.17%	0.017%
43	13.993	1830	1837	1847	rBV	3352034	4690167	40.32%	4.041%
44	14.234	1873	1878	1879	rBV5	14400	16845	0.14%	0.015%
45	14.281	1879	1886	1897	rVB	3695630	5387528	46.31%	4.642%
46	14.422	1906	1910	1916	rVV7	10201	14477	0.12%	0.012%
47	14.587	1931	1938	1947	rVB	2779788	4038259	34.71%	3.479%
48	14.781	1965	1971	1988	rBV	310163	543712	4.67%	0.468%
49	14.934	1992	1997	2004	rVV	75517	121325	1.04%	0.105%
50	14.993	2004	2007	2011	rVB5	14452	19874	0.17%	0.017%
51	15.322	2059	2063	2067	rBV	21539	27609	0.24%	0.024%
52	15.575	2099	2106	2116	rBV	4849205	7061700	60.70%	6.084%
53	15.692	2120	2126	2141	rVV	1798010	2389945	20.54%	2.059%
54	15.810	2142	2146	2155	rVB3	25986	46818	0.40%	0.040%
55	15.940	2163	2168	2175	rBV	362739	504892	4.34%	0.435%
56	16.287	2223	2227	2231	rVB2	17803	24238	0.21%	0.021%
57	16.722	2296	2301	2311	rBV2	53855	80042	0.69%	0.069%
58	17.010	2347	2350	2357	rVB9	10715	15683	0.13%	0.014%
59	17.081	2357	2362	2365	rBV4	9603	15360	0.13%	0.013%
60	17.122	2365	2369	2373	rBV3	9754	15932	0.14%	0.014%
61	17.334	2398	2405	2414	rBV	3454086	4899519	42.11%	4.221%
62	17.434	2415	2422	2431	rBV2	6123022	8782568	75.49%	7.567%
63	17.592	2444	2449	2450	rBV5	12190	18349	0.16%	0.016%
64	17.710	2465	2469	2472	rBV3	11351	16206	0.14%	0.014%
65	18.098	2530	2535	2540	rBV8	11851	25858	0.22%	0.022%
66	18.234	2551	2558	2602	rBV	7181810	10752798	92.43%	9.264%
67	18.716	2637	2640	2646	rVB6	18283	27535	0.24%	0.024%
68	18.981	2683	2685	2689	rVB4	18643	20674	0.18%	0.018%
69	19.292	2733	2738	2744	rVB2	82701	118034	1.01%	0.102%
70	19.381	2744	2753	2755	rBV3	369275	683106	5.87%	0.589%
71	19.498	2768	2773	2790	rBV	1182351	1627286	13.99%	1.402%
72	19.728	2806	2812	2820	rBV	7799771	10634252	91.41%	9.162%
73	20.192	2886	2891	2895	rBV4	62131	107656	0.93%	0.093%
74	20.257	2898	2902	2904	rBV2	101712	152207	1.31%	0.131%
75	20.592	2955	2959	2963	rBV2	81637	123250	1.06%	0.106%
76	20.692	2972	2976	2983	rBV2	287667	444825	3.82%	0.383%

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77	21.192	3057	3061	3077	rBV2	594816	1356494	11.66%	1.169%
78	21.363	3087	3090	3093	rBV2	93711	116712	1.00%	0.101%
79	21.522	3111	3117	3123	rBV	4185466	5639110	48.47%	4.858%
80	22.127	3217	3220	3230	rBV2	137484	236580	2.03%	0.204%
81	22.280	3242	3246	3251	rBV	420522	640168	5.50%	0.552%
82	22.416	3266	3269	3275	rBV2	206497	341946	2.94%	0.295%
83	22.639	3303	3307	3315	rVB	221265	408867	3.51%	0.352%
84	22.774	3327	3330	3338	rVB	323190	476099	4.09%	0.410%
85	23.192	3398	3401	3411	rVB2	197483	322988	2.78%	0.278%
86	23.804	3497	3505	3519	rVB2	5685690	11633714	100.00%	10.023%
87	23.957	3524	3531	3545	rVB	2765167	5758786	49.50%	4.961%
88	24.563	3630	3634	3642	rVB	268081	527265	4.53%	0.454%

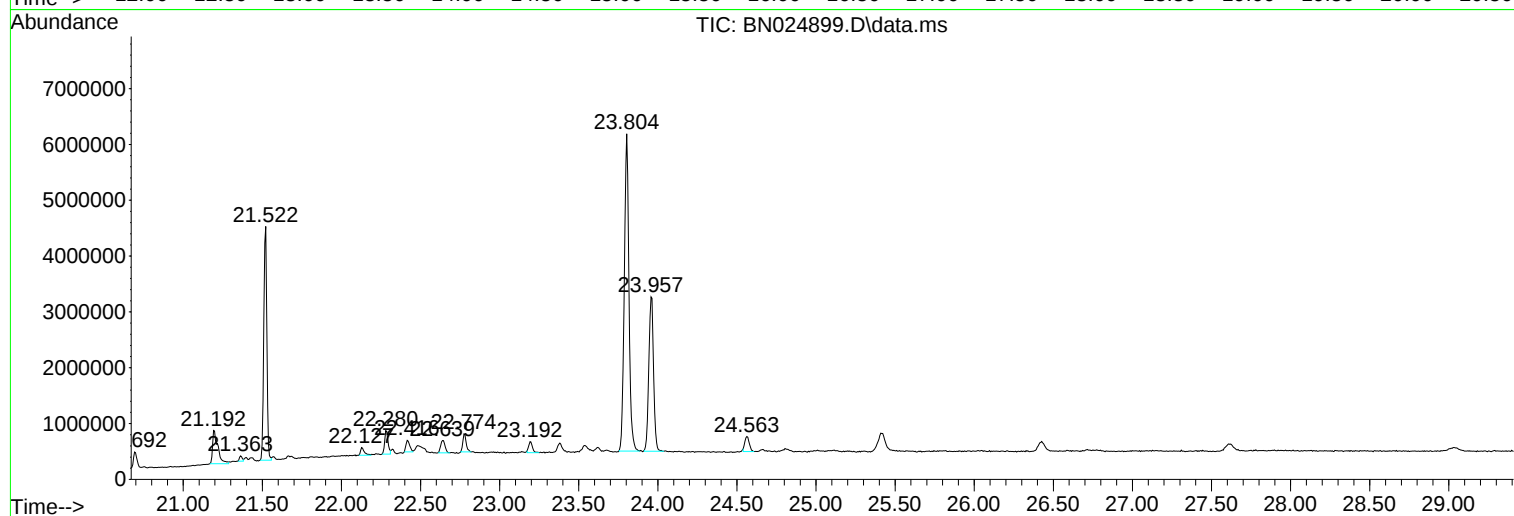
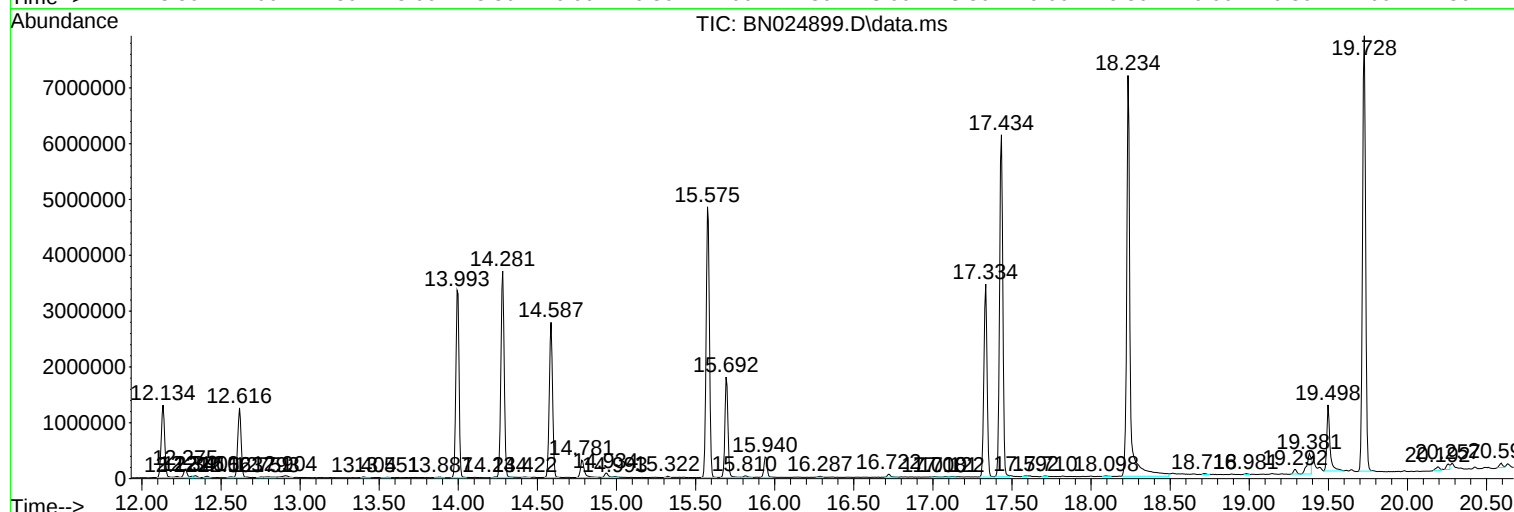
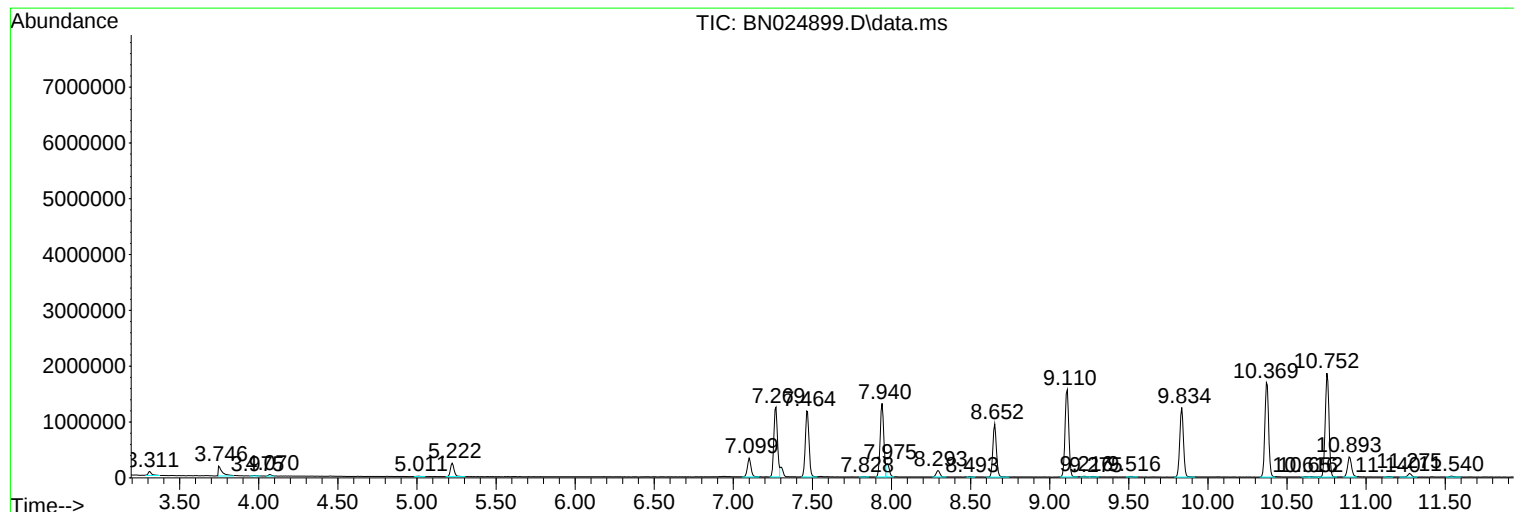
Sum of corrected areas: 116071335

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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



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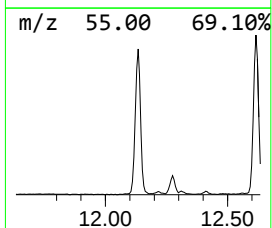
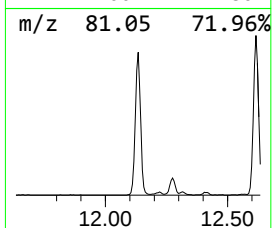
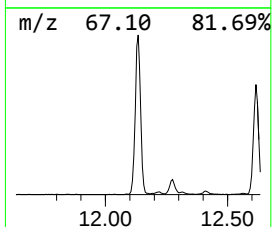
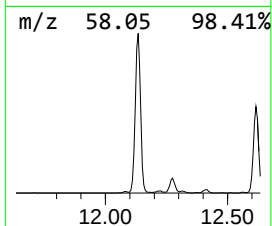
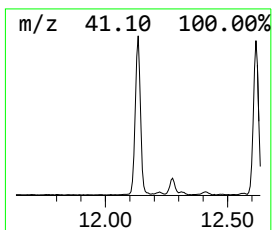
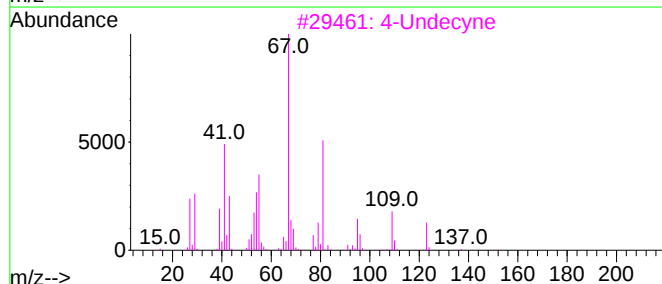
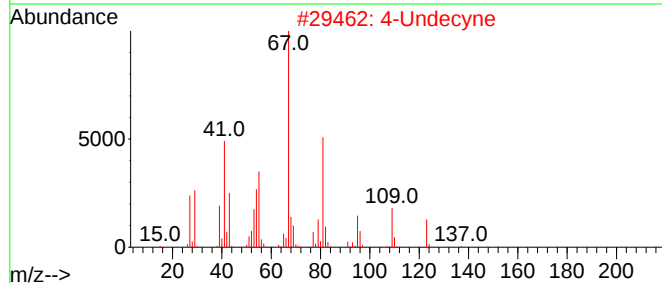
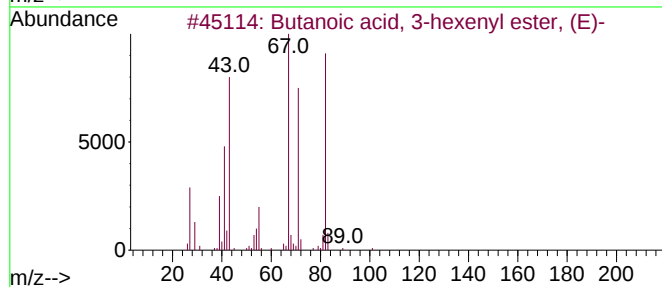
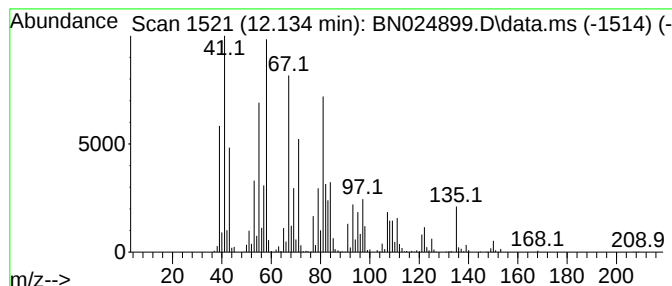
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.134	12.88 ng/ul	1970490	Naphthalene-d8	10.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hexenyl ester, ...	170	C10H18O2	053398-84-8	27
2			4-Undecyne	152	C11H20	060212-31-9	18
3			4-Undecyne	152	C11H20	060212-31-9	18
4			7-Formylbicyclo[4.1.0]heptane	124	C8H12O	1000197-01-8	18
5			1,2-Oxathiolane, 2,2-dioxide	122	C3H6O3S	001120-71-4	18



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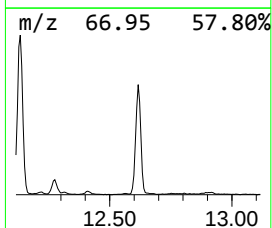
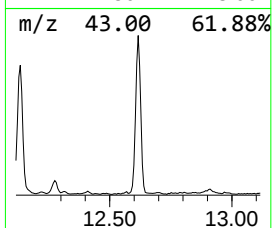
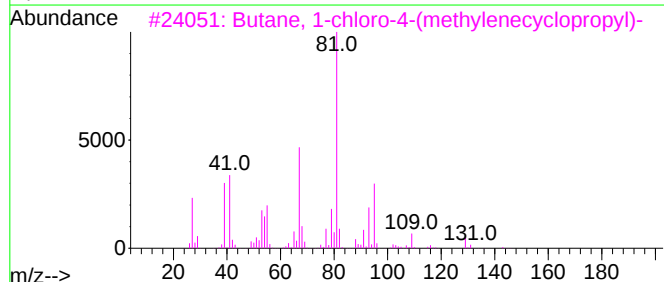
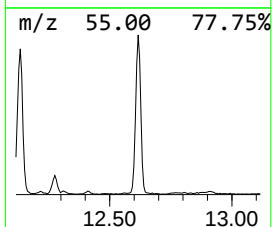
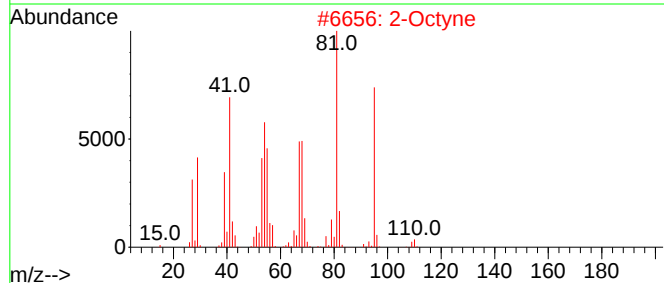
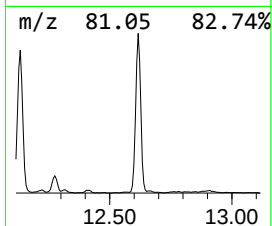
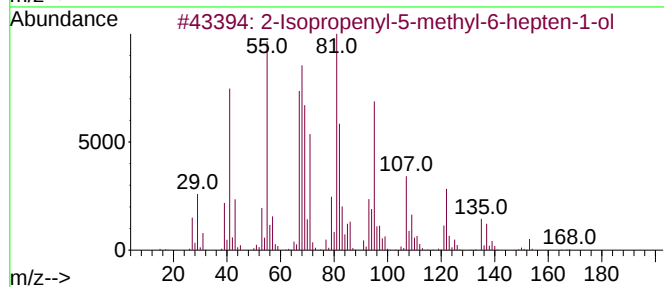
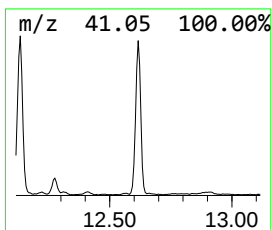
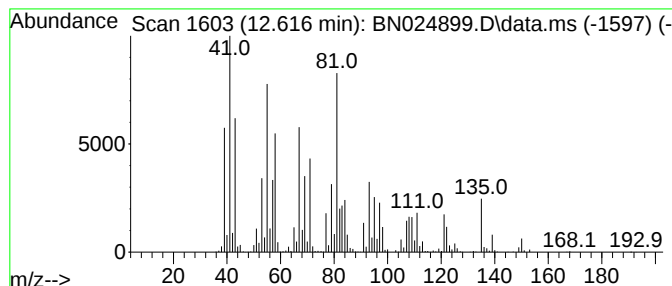
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	11.82 ng/ul	1808160	Naphthalene-d8	10.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropenyl-5-methyl-6-hepten-...	168	C11H20O	013066-55-2	47		
2	2-Octyne	110	C8H14	002809-67-8	38		
3	Butane, 1-chloro-4-(methylenecyc...	144	C8H13Cl	1000158-48-9	35		
4	1,8-Nonadiene, 2,8-dimethyl-	152	C11H20	020054-25-5	35		
5	trans-(2-Ethylcyclopentyl)methanol	128	C8H16O	036258-08-9	27		



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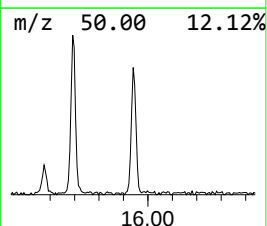
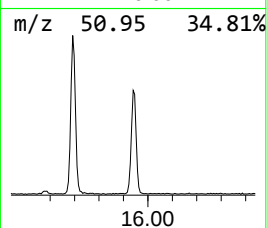
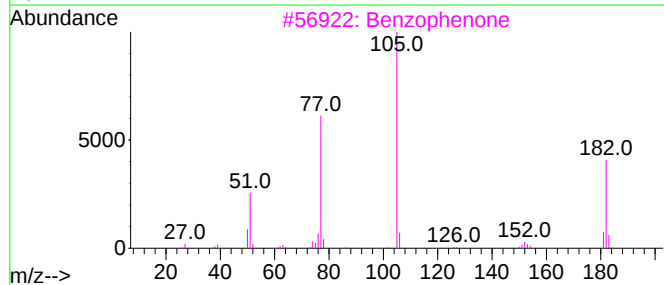
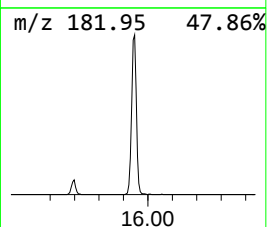
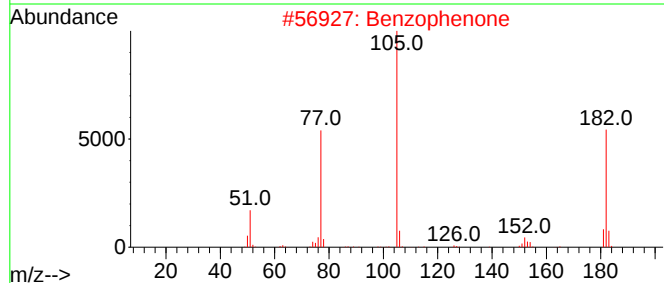
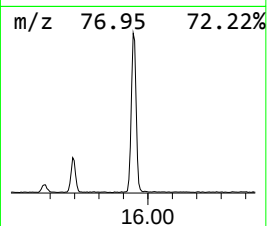
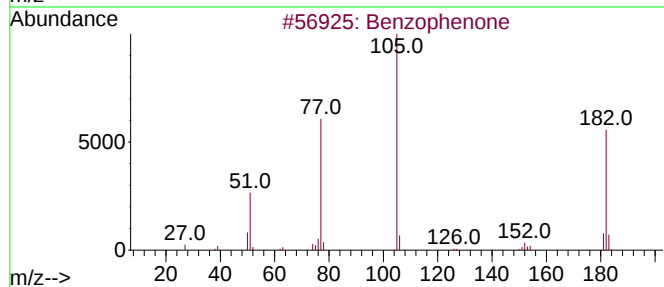
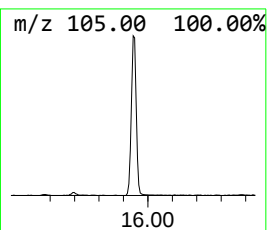
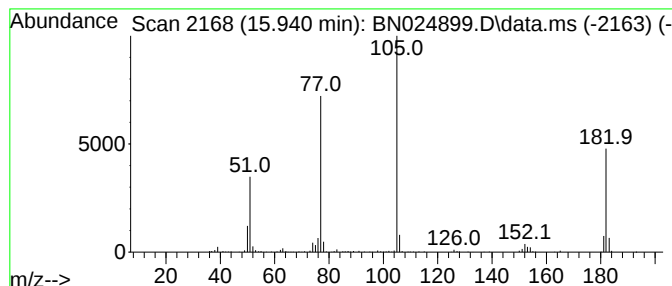
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.940	2.50 ng/ul	504892	Acenaphthene-d10	14.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	97
3			Benzophenone	182	C13H10O	000119-61-9	96
4			Benzophenone	182	C13H10O	000119-61-9	91
5			Benzophenone	182	C13H10O	000119-61-9	87



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Misc :
ALS Vial : 45 Sample Multiplier: 1

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ClientSampleId :
COME3

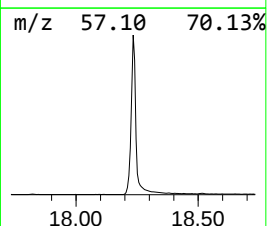
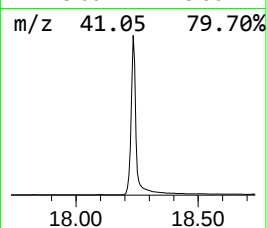
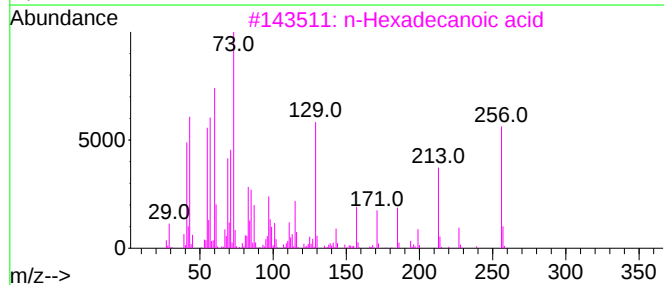
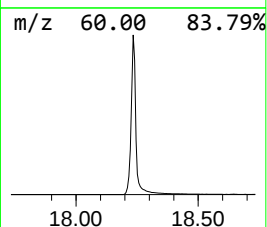
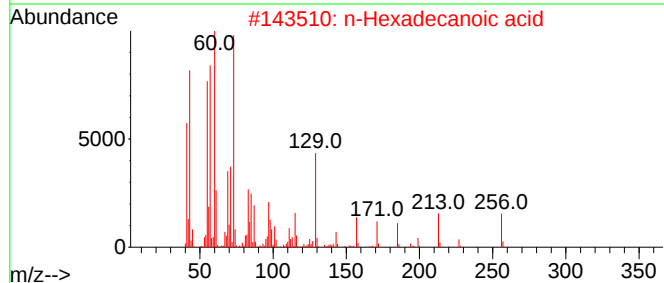
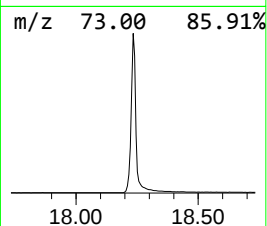
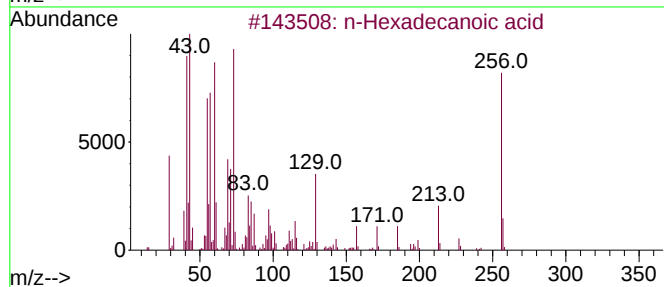
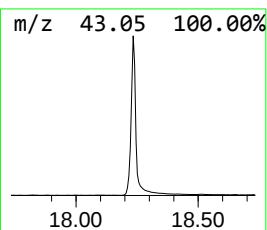
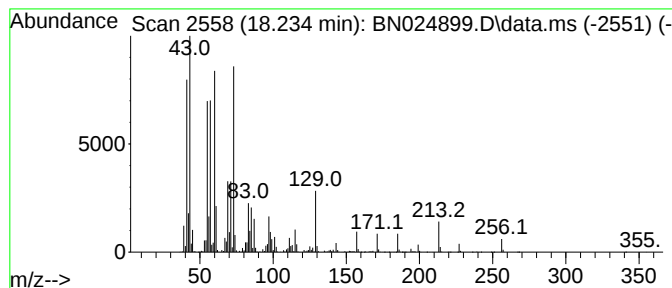
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	43.89 ng/ul	10752800	Phenanthrene-d10	17.334

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	96
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024899.D
Acq On : 14 Apr 2023 15:54
Operator : CG/JU
Sample : 02252-07
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COME3

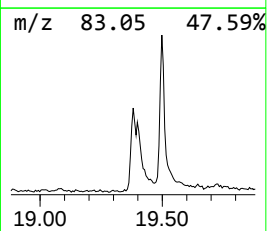
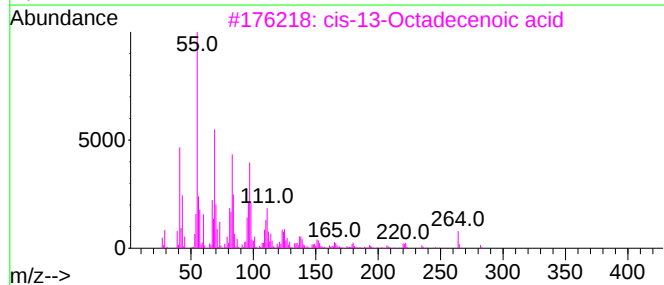
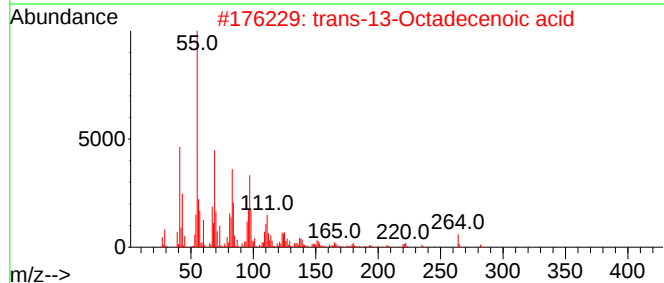
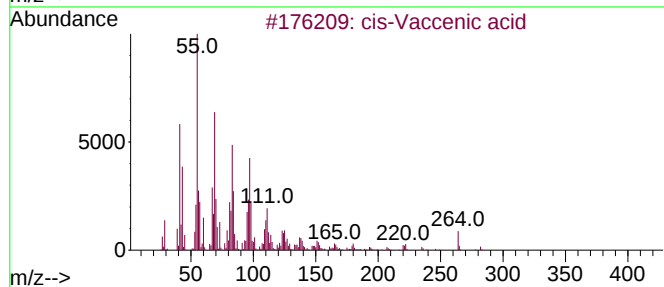
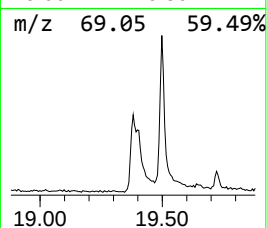
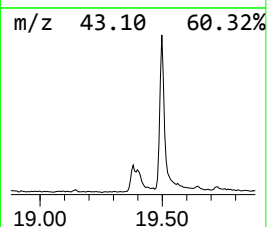
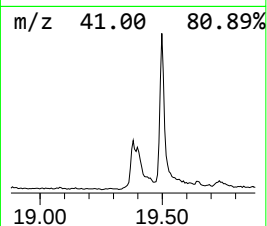
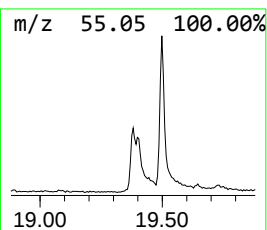
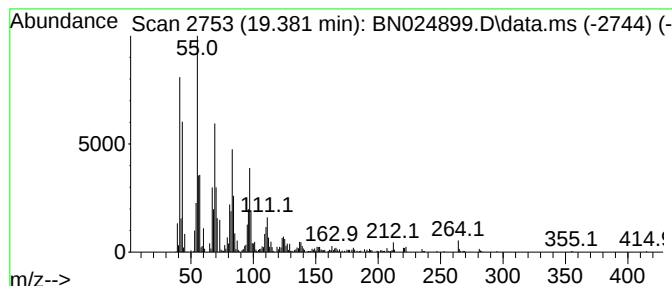
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 cis-Vaccenic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.381	2.79 ng/ul	683106	Phenanthrene-d10	17.334

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	98
2			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	97
3			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	97
4			Heptadecanolide	268	C17H32O2	005637-97-8	92
5			9-Octadecenoic acid	282	C18H34O2	002027-47-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024899.D
Acq On : 14 Apr 2023 15:54
Operator : CG/JU
Sample : 02252-07
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COME3

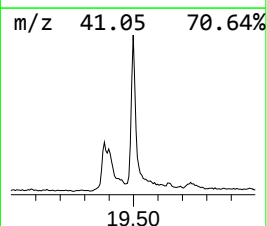
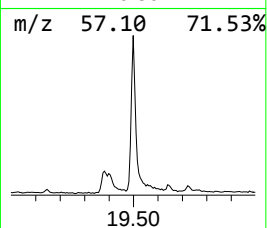
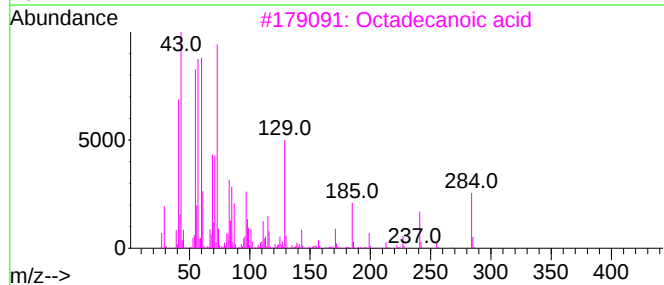
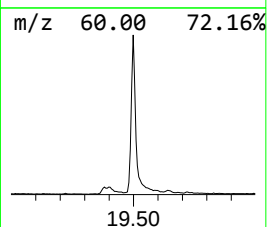
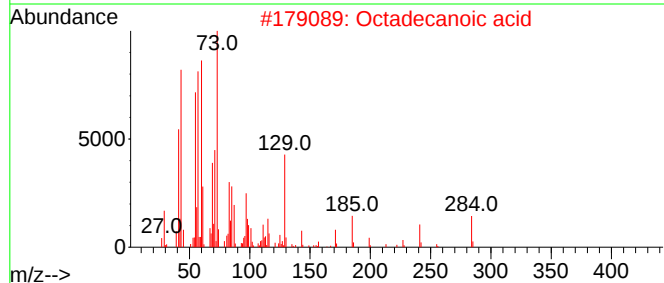
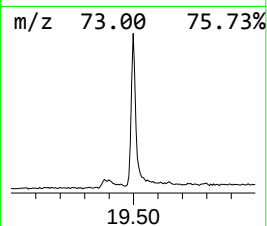
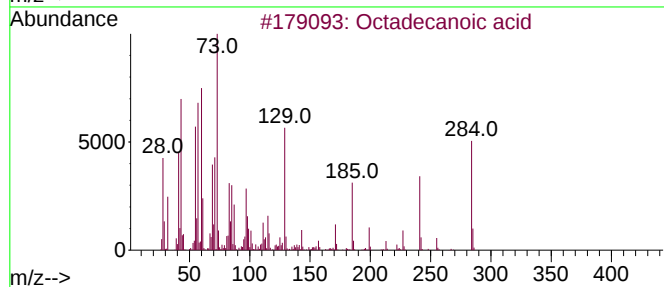
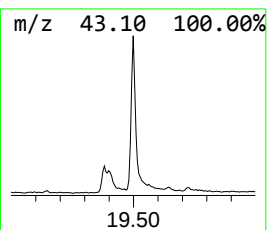
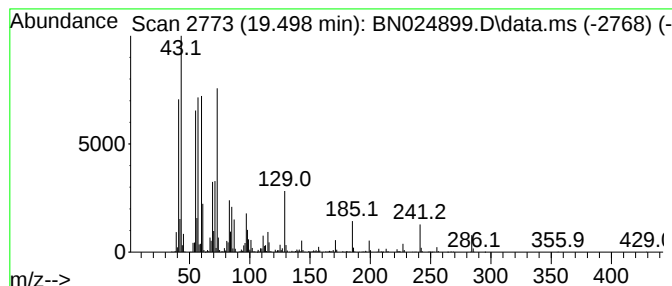
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.498	5.77 ng/ul	1627290	Chrysene-d12	21.522

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	95
4			Octadecanoic acid	284	C18H36O2	000057-11-4	94
5			Octadecanoic acid	284	C18H36O2	000057-11-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024899.D
Acq On : 14 Apr 2023 15:54
Operator : CG/JU
Sample : 02252-07
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COME3

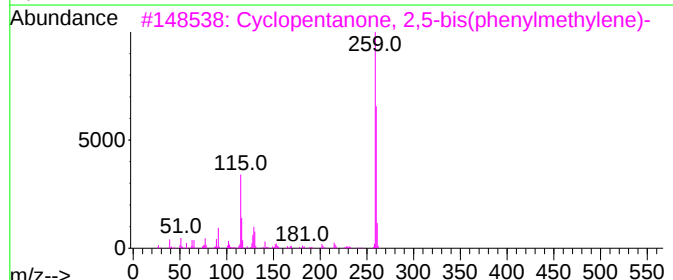
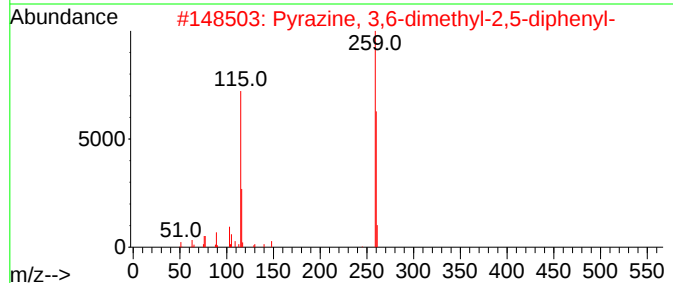
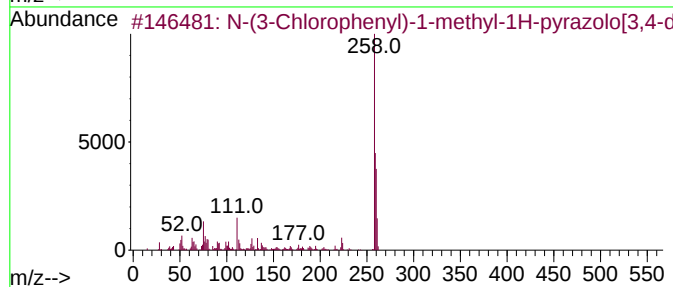
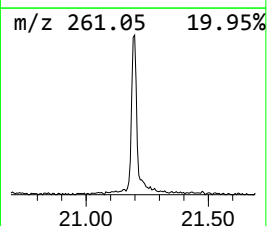
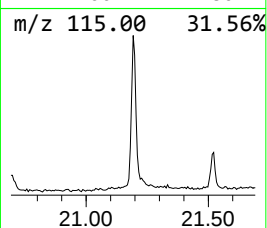
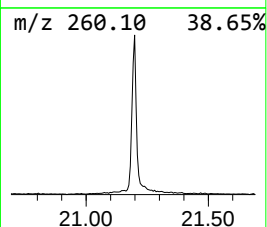
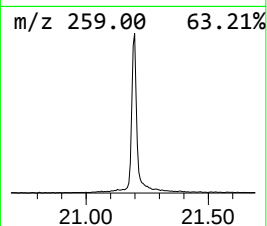
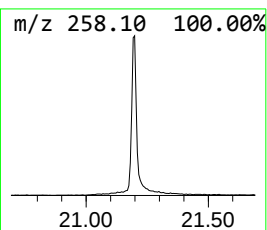
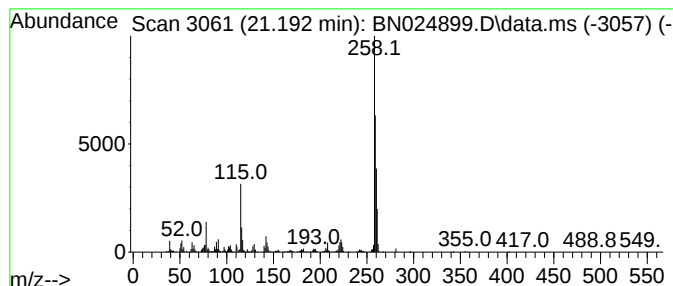
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 N-(3-Chlorophenyl)-1-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	4.81 ng/ul	1356490	Chrysene-d12	21.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(3-Chlorophenyl)-1-methyl-1H-p...	259	C12H10ClN5	1000486-15-0	81
2			Pyrazine, 3,6-dimethyl-2,5-diphe...	260	C18H16N2	1000298-55-3	43
3			Cyclopentanone, 2,5-bis(phenylme...	260	C19H16O	000895-80-7	38
4			4-Amino-3-[p-chlorophenyl]-1-met...	259	C12H10ClN5	058791-75-6	38
5			2,3',6-Trichlorobiphenyl	256	C12H7Cl3	038444-76-7	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024899.D
Acq On : 14 Apr 2023 15:54
Operator : CG/JU
Sample : 02252-07
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COME3

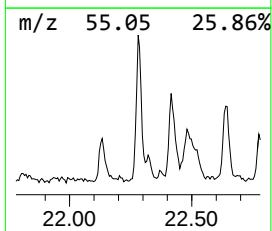
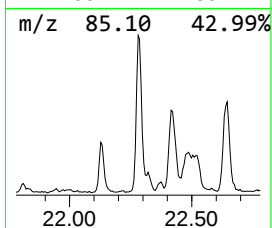
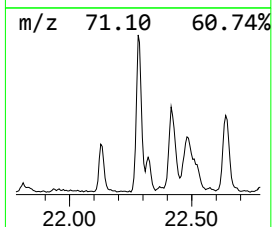
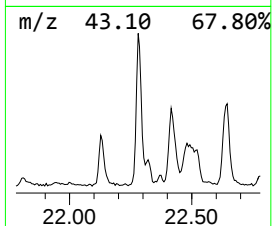
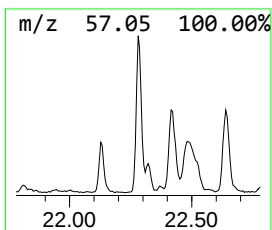
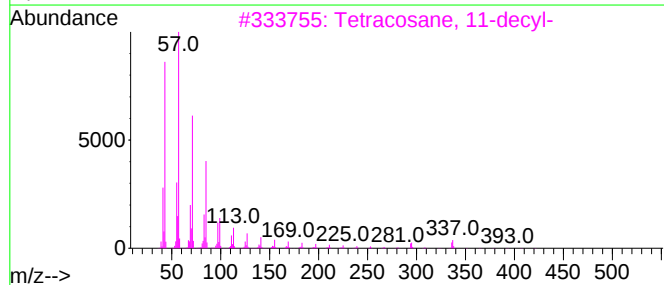
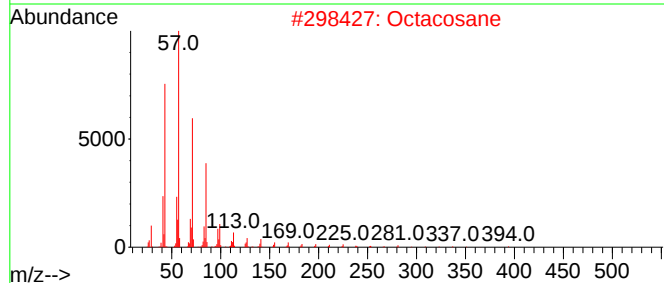
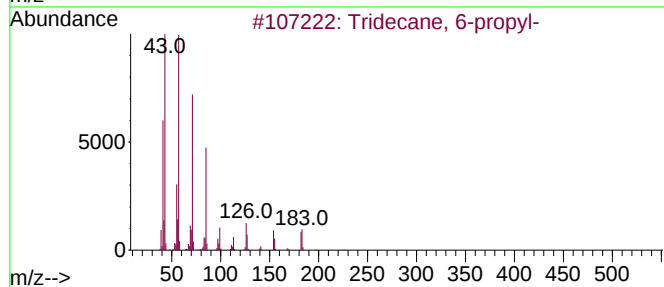
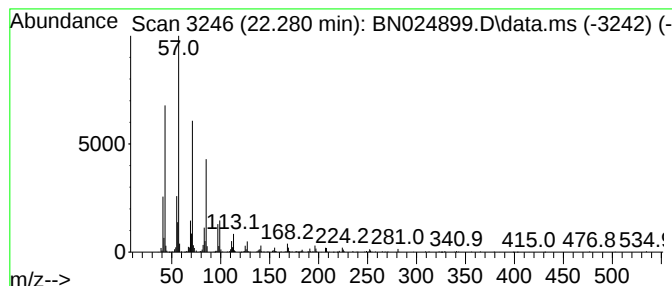
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.280	2.27 ng/ul	640168	Chrysene-d12	21.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 6-propyl-	226	C16H34	055045-10-8	91
2			Octacosane	394	C28H58	000630-02-4	90
3			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	87
4			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	87
5			Heptacosane	380	C27H56	000593-49-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN041423\
Data File : BN024899.D
Acq On : 14 Apr 2023 15:54
Operator : CG/JU
Sample : 02252-07
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
COME3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN041023.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
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unknown-02	12.616	11.8	ng/ul	1808160	2	10.752	3060700	20.0
Benzophenone	15.940	2.5	ng/ul	504892	3	14.587	4038260	20.0
n-Hexadecanoic ...	18.233	43.9	ng/ul	10752800	4	17.334	4899520	20.0
cis-Vaccenic acid	19.381	2.8	ng/ul	683106	4	17.334	4899520	20.0
Octadecanoic acid	19.498	5.8	ng/ul	1627290	5	21.522	5639110	20.0
N-(3-Chlorophen...	21.192	4.8	ng/ul	1356490	5	21.522	5639110	20.0
(DEL) Alkane: S...	22.280	2.3	ng/ul	640168	5	21.522	5639110	20.0