

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
 Data File : BG059518.D
 Acq On : 28 Oct 2023 12:26
 Operator : MA/JU
 Sample : 04925-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GCCW9

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_G\Methods\SFAM-EPA-BG102723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BG059518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.661	41	46	48	rBV2	13422	19923	1.29%	0.124%
2	3.796	66	69	72	rBV2	6524	6793	0.44%	0.042%
3	3.925	89	91	92	rBV2	7421	4353	0.28%	0.027%
4	4.096	116	120	124	rBV3	16082	28064	1.82%	0.175%
5	4.219	135	141	146	rBV4	15735	24374	1.58%	0.152%
6	4.313	152	157	160	rBV	14305	21774	1.41%	0.136%
7	4.366	163	166	168	rBV2	4098	4623	0.30%	0.029%
8	4.431	174	177	180	rBV3	4859	5636	0.37%	0.035%
9	4.489	185	187	189	rBV2	5206	5151	0.33%	0.032%
10	4.578	198	202	205	rBV4	3028	5044	0.33%	0.031%
11	4.754	230	232	239	rVB2	6523	11702	0.76%	0.073%
12	4.807	239	241	242	rBV	8050	5962	0.39%	0.037%
13	5.265	317	319	324	rBV2	4797	7296	0.47%	0.045%
14	5.377	333	338	341	rVB2	25683	36526	2.37%	0.227%
15	5.459	349	352	353	rBV2	7139	6209	0.40%	0.039%
16	5.641	381	383	386	rBV4	6120	6131	0.40%	0.038%
17	6.046	448	452	454	rVB2	4400	4571	0.30%	0.028%
18	6.575	538	542	545	rBV	4064	5932	0.38%	0.037%
19	6.652	553	555	558	rBV	6477	7992	0.52%	0.050%
20	6.781	575	577	579	rVB2	6329	4401	0.29%	0.027%
21	6.822	582	584	587	rVB	4880	5218	0.34%	0.032%
22	6.975	607	610	611	rBV2	8266	9249	0.60%	0.058%
23	7.022	617	618	623	rBV4	4814	5136	0.33%	0.032%
24	7.321	666	669	671	rBV3	6598	5542	0.36%	0.034%
25	7.339	671	672	675	rVB2	7700	6323	0.41%	0.039%
26	7.468	687	694	705	rBV	240162	458494	29.75%	2.854%
27	7.680	724	730	738	rVV	179001	306169	19.87%	1.906%
28	7.762	742	744	750	rVB5	12125	14473	0.94%	0.090%
29	7.874	757	763	769	rBV	241490	424387	27.54%	2.641%
30	8.244	824	826	829	rBV3	6430	10247	0.66%	0.064%
31	8.361	840	846	853	rVB	218017	368837	23.94%	2.296%
32	8.520	870	873	876	rBV4	4304	5797	0.38%	0.036%
33	8.585	883	884	889	rVB3	4617	6100	0.40%	0.038%
34	8.649	889	895	899	rBV6	15154	25684	1.67%	0.160%
35	8.761	912	914	916	rBV3	5607	5404	0.35%	0.034%
36	8.837	923	927	930	rBV2	4122	7202	0.47%	0.045%

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37	9.043	956	962	968	rVB2	262186	484102	31.42%	3.013%
38	9.108	972	973	975	rBV2	6471	5612	0.36%	0.035%
39	9.207	985	990	998	rVB	89362	162685	10.56%	1.013%
40	9.560	1042	1050	1056	rBV2	183877	351876	22.84%	2.190%

41	9.783	1084	1088	1089	rBV2	5893	6023	0.39%	0.037%
42	9.860	1098	1101	1102	rBV	4853	5092	0.33%	0.032%
43	10.277	1166	1172	1179	rBV	144744	260412	16.90%	1.621%
44	10.477	1204	1206	1209	rVB2	5518	4471	0.29%	0.028%
45	10.641	1232	1234	1239	rVB2	14141	17352	1.13%	0.108%

46	10.800	1255	1261	1274	rVB2	303161	557073	36.15%	3.467%
47	10.947	1283	1286	1287	rBV2	6450	5392	0.35%	0.034%
48	10.958	1287	1288	1289	rBV	8800	4500	0.29%	0.028%
49	11.070	1306	1307	1310	rBV	6447	5761	0.37%	0.036%
50	11.111	1313	1314	1320	rVB4	6258	7916	0.51%	0.049%

51	11.211	1322	1331	1342	rVV	291542	577143	37.45%	3.592%
52	11.352	1349	1355	1367	rVB3	89552	184395	11.97%	1.148%
53	11.722	1416	1418	1419	rBV2	10520	5768	0.37%	0.036%
54	11.769	1424	1426	1428	rBV	5648	5654	0.37%	0.035%
55	11.898	1447	1448	1452	rVB	6480	4789	0.31%	0.030%

56	12.051	1470	1474	1475	rBV2	4410	5963	0.39%	0.037%
57	12.216	1499	1502	1507	rVB2	7141	11507	0.75%	0.072%
58	12.551	1557	1559	1562	rBV4	5022	4648	0.30%	0.029%
59	12.768	1593	1596	1599	rVB3	6972	7917	0.51%	0.049%
60	12.833	1605	1607	1611	rBV	4589	4535	0.29%	0.028%

61	12.921	1619	1622	1624	rBV2	4455	5082	0.33%	0.032%
62	13.162	1661	1663	1666	rBV2	7459	5968	0.39%	0.037%
63	13.279	1679	1683	1685	rBV4	4003	6130	0.40%	0.038%
64	13.690	1751	1753	1755	rBV	4856	5020	0.33%	0.031%
65	13.831	1770	1777	1783	rBV2	108818	190917	12.39%	1.188%

66	14.025	1805	1810	1813	rBV2	5931	8715	0.57%	0.054%
67	14.108	1822	1824	1828	rBV5	15297	22461	1.46%	0.140%
68	14.172	1830	1835	1837	rVV3	7658	13280	0.86%	0.083%
69	14.243	1842	1847	1851	rBV7	25526	43623	2.83%	0.271%
70	14.331	1861	1862	1865	rBV3	5702	4309	0.28%	0.027%

71	14.384	1865	1871	1882	rVB	586704	853349	55.38%	5.311%
72	14.554	1898	1900	1903	rBV2	4232	4398	0.29%	0.027%
73	14.695	1917	1924	1930	rBV	634185	1042747	67.67%	6.490%
74	14.772	1935	1937	1939	rVV2	6328	4450	0.29%	0.028%
75	14.848	1948	1950	1953	rVB2	8270	7087	0.46%	0.044%

76	14.907	1956	1960	1964	rVB5	14554	19393	1.26%	0.121%
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77	14.995	1968	1975	1982	rVV	453900	735216	47.71%	4.576%
78	15.148	1994	2001	2008	rBV2	230907	380355	24.68%	2.367%
79	15.247	2012	2018	2028	rVV3	117975	214074	13.89%	1.332%
80	15.336	2028	2033	2040	rVB6	33441	59213	3.84%	0.369%
81	15.394	2040	2043	2045	rBV3	8269	8993	0.58%	0.056%
82	15.488	2057	2059	2062	rVB	8248	8359	0.54%	0.052%
83	15.706	2091	2096	2100	rVB4	12319	21799	1.41%	0.136%
84	15.929	2132	2134	2135	rBV	6658	4991	0.32%	0.031%
85	15.976	2136	2142	2151	rVB	819232	1273976	82.68%	7.929%
86	16.076	2154	2159	2165	rBV2	149907	236330	15.34%	1.471%
87	16.669	2258	2260	2268	rVB9	13088	25106	1.63%	0.156%
88	17.568	2410	2413	2418	rVV6	40525	51378	3.33%	0.320%
89	17.633	2421	2424	2429	rVB4	42959	54922	3.56%	0.342%
90	17.745	2437	2443	2450	rVB	585193	931733	60.47%	5.799%
91	17.844	2453	2460	2467	rBV	859315	1352789	87.79%	8.419%
92	18.350	2544	2546	2553	rVB7	17331	23784	1.54%	0.148%
93	18.455	2559	2564	2568	rBV6	27232	52109	3.38%	0.324%
94	18.514	2571	2574	2579	rVV3	93714	119449	7.75%	0.743%
95	18.573	2579	2584	2594	rVV	335658	465596	30.22%	2.898%
96	19.830	2794	2798	2806	rVB2	123322	172089	11.17%	1.071%
97	20.112	2840	2846	2852	rBV2	1077284	1540910	100.00%	9.590%
98	20.958	2986	2990	2994	rVB2	168142	217489	14.11%	1.354%
99	21.640	3102	3106	3112	rBV2	330828	442350	28.71%	2.753%
100	22.081	3176	3181	3189	rVB2	473924	860170	55.82%	5.354%

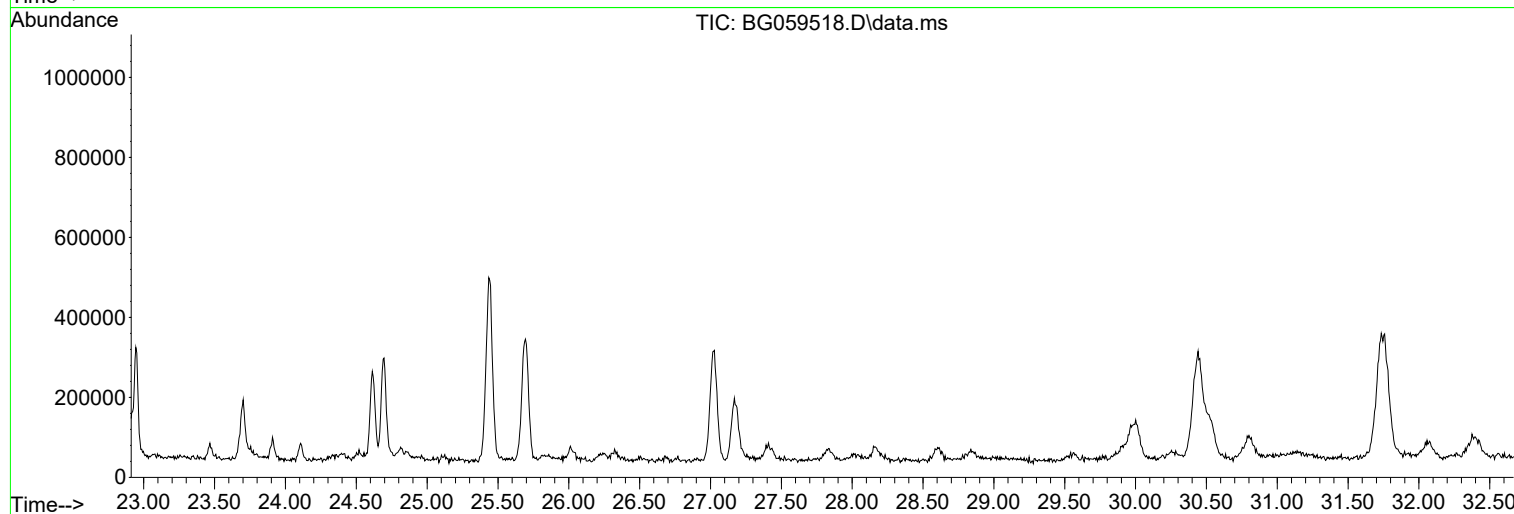
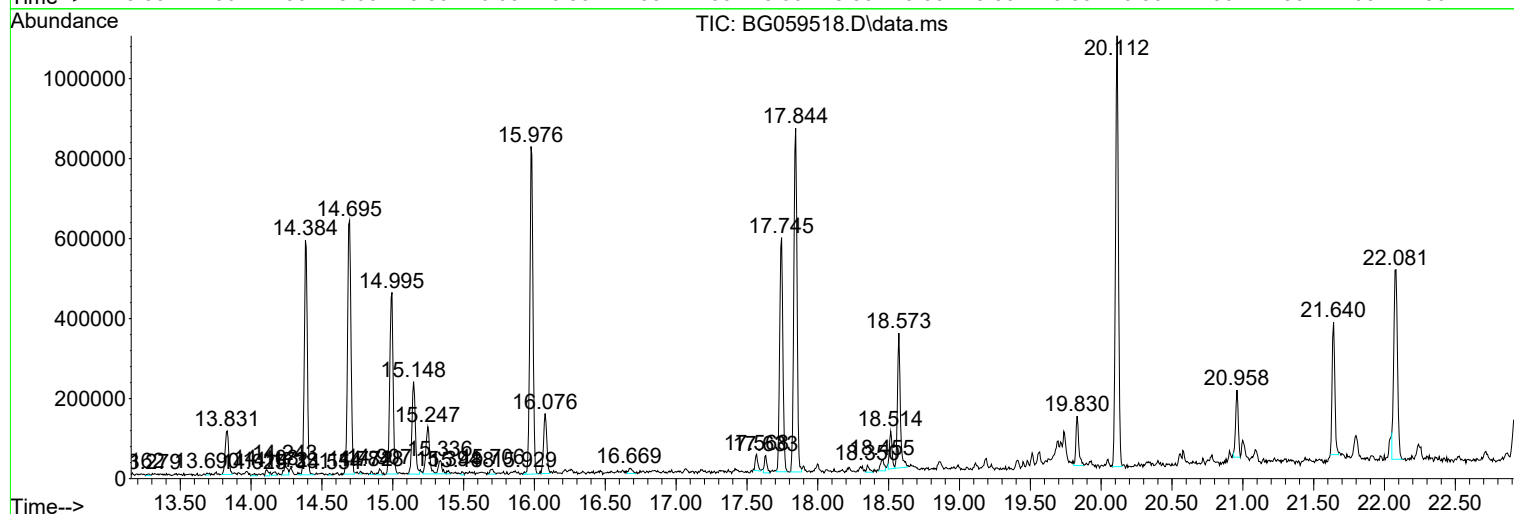
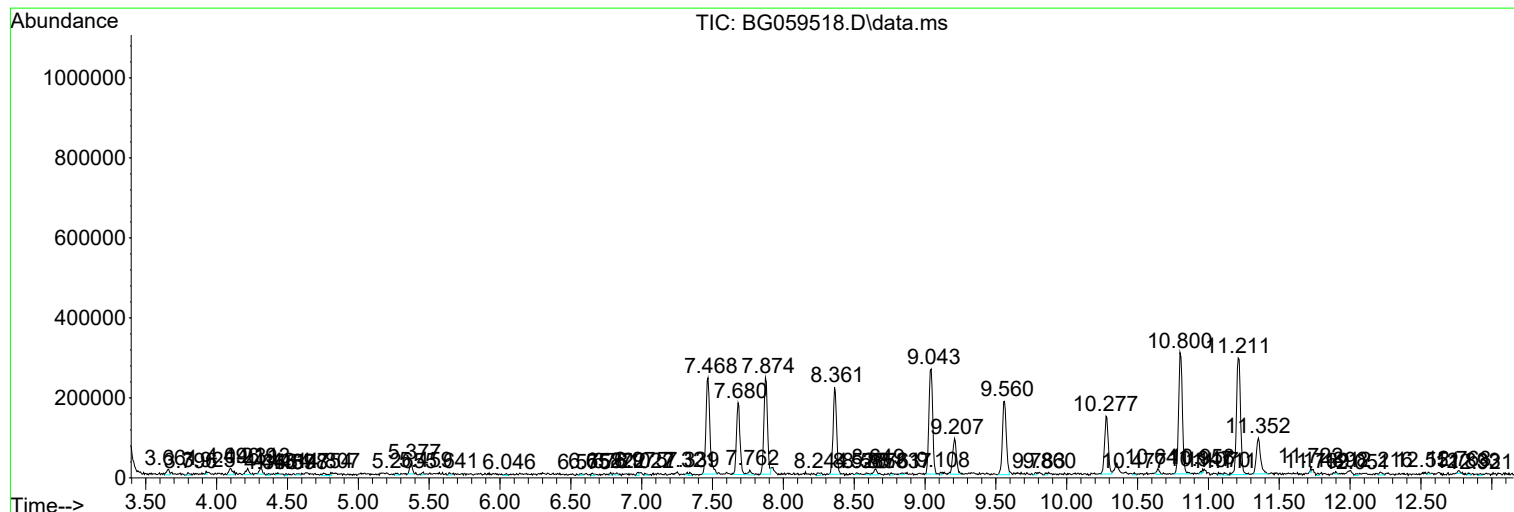
Sum of corrected areas: 16067414

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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



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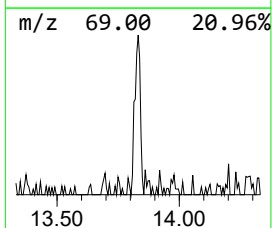
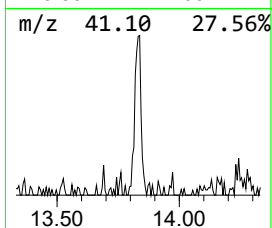
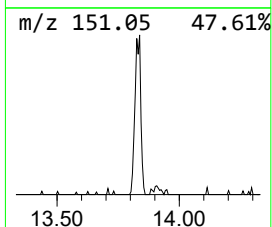
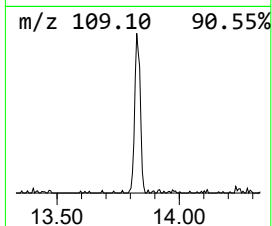
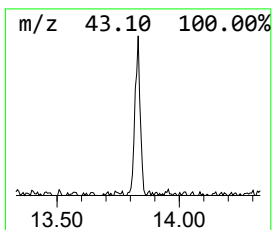
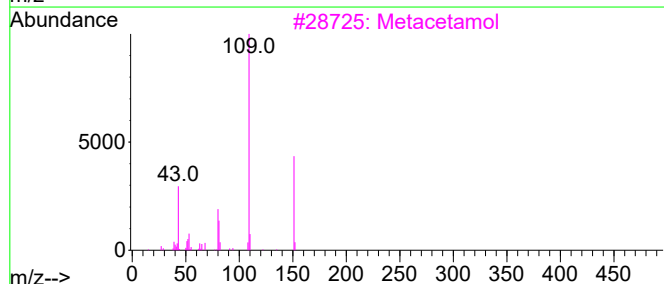
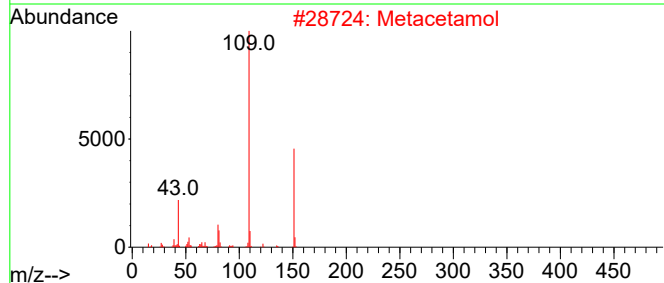
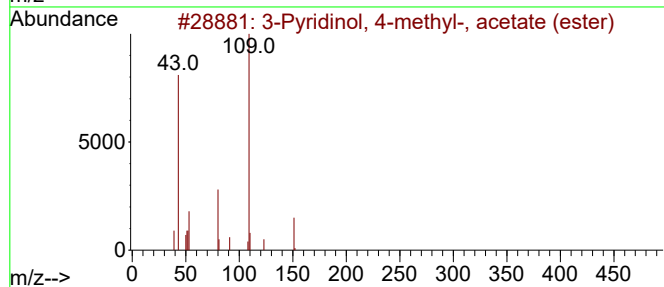
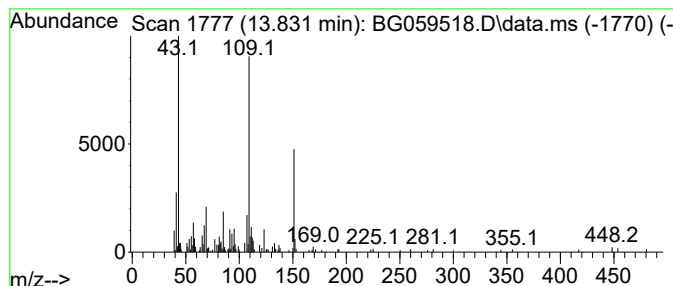
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 3-Pyridinol, 4-methyl-, ace... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.832	5.19 ng/ul	190917	Acenaphthene-d10	14.995

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
2			Metacetamol	151	C8H9NO2	000621-42-1	58
3			Metacetamol	151	C8H9NO2	000621-42-1	58
4			Acetaminophen	151	C8H9NO2	000103-90-2	53
5			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53



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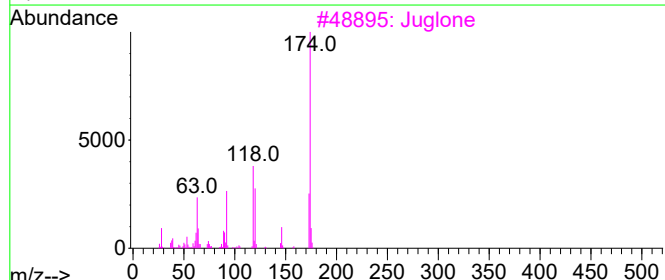
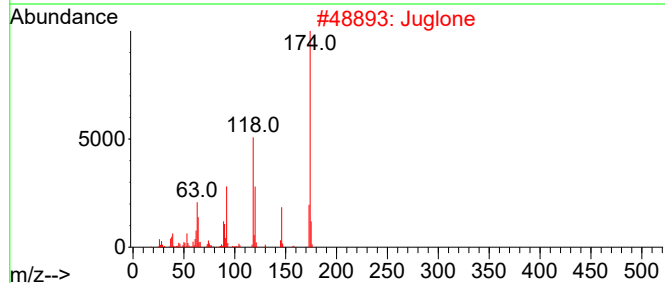
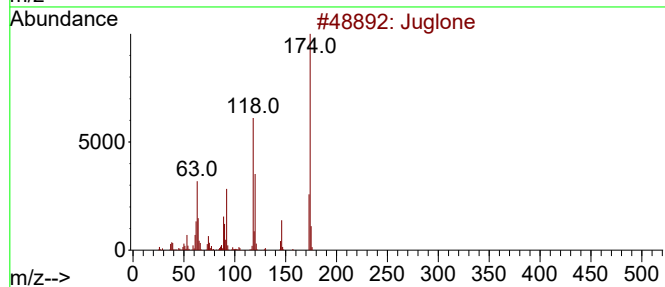
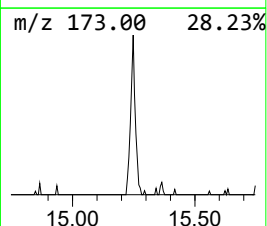
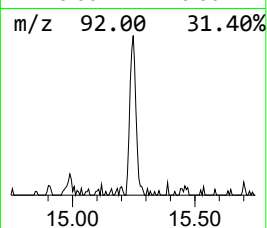
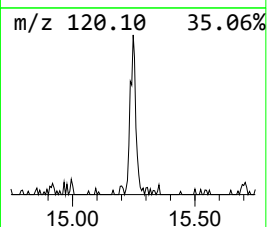
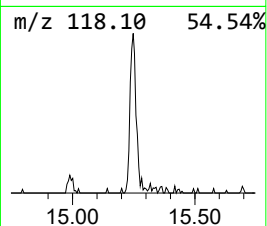
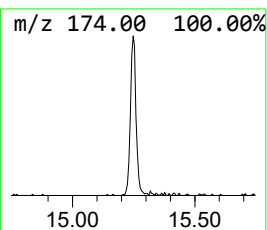
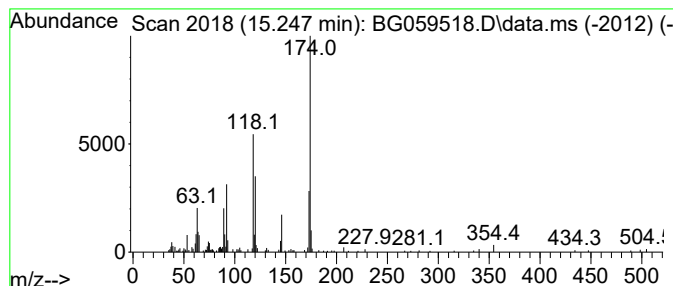
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Juglone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.248	5.82 ng/ul	214074	Acenaphthene-d10	14.995

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Juglone			174	C10H6O3	000481-39-0	93
2	Juglone			174	C10H6O3	000481-39-0	93
3	Juglone			174	C10H6O3	000481-39-0	93
4	Juglone			174	C10H6O3	000481-39-0	91
5	Benzene, 2,4-diisocyanato-1-methyl-			174	C9H6N2O2	000584-84-9	43



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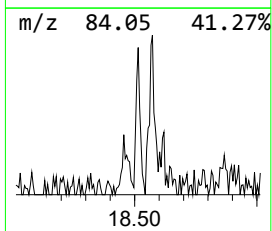
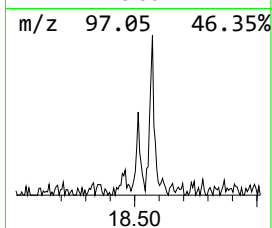
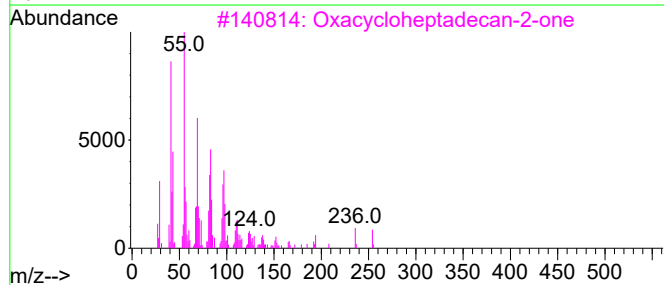
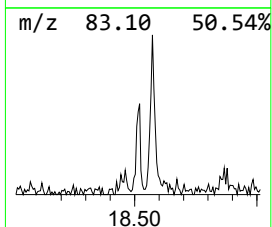
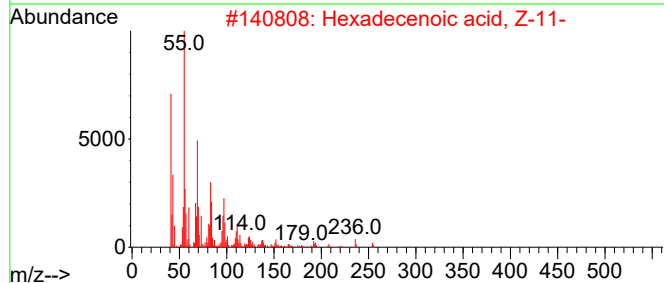
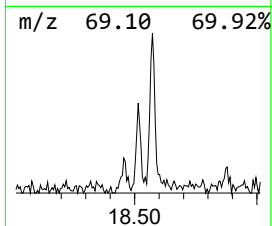
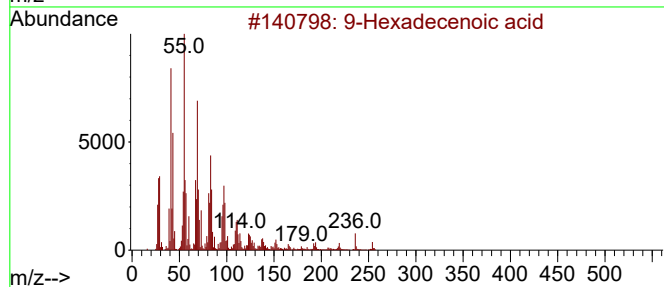
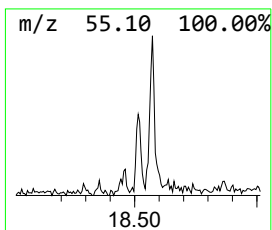
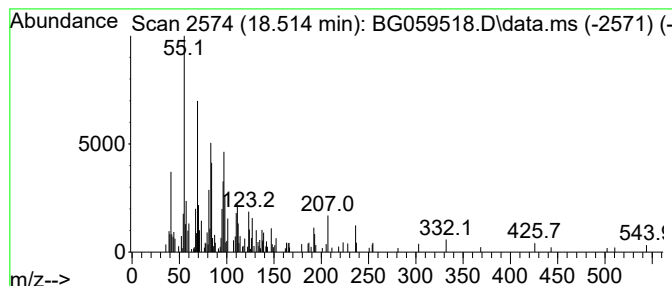
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 9-Hexadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.514	2.56 ng/ul	119449	Phenanthrene-d10		17.744	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid		254	C16H30O2	002091-29-4	91
2	Hexadecenoic acid, Z-11-		254	C16H30O2	002416-20-8	90
3	Oxacycloheptadecan-2-one		254	C16H30O2	000109-29-5	83
4	Butyl 9-hexadecenoate		310	C20H38O2	1000336-51-9	83
5	cis-7-Hexadecenoic acid		254	C16H30O2	002416-19-5	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059518.D
Acq On : 28 Oct 2023 12:26
Operator : MA/JU
Sample : 04925-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCW9

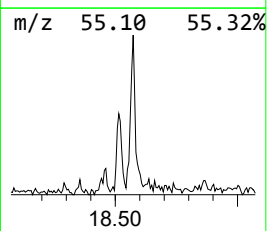
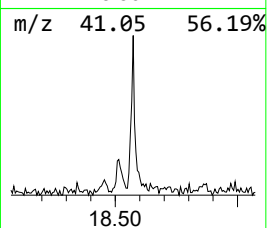
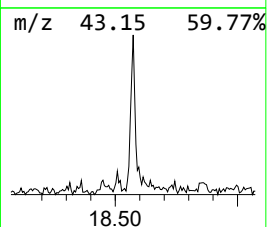
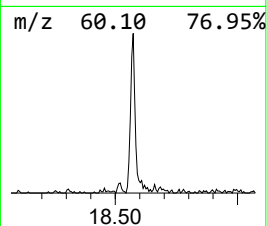
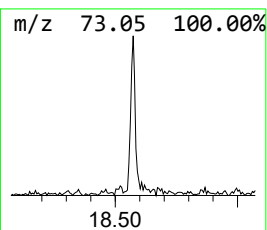
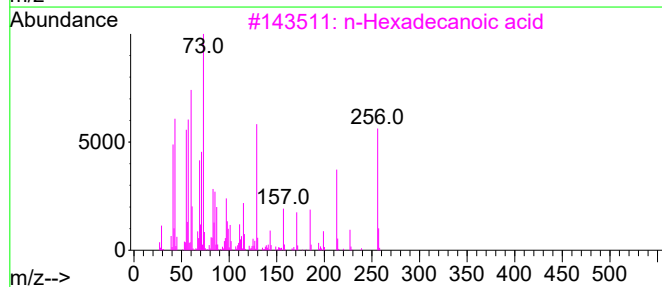
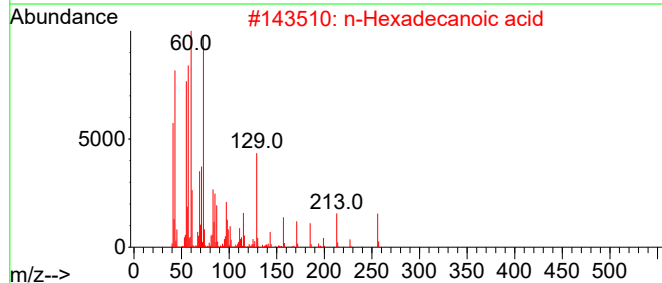
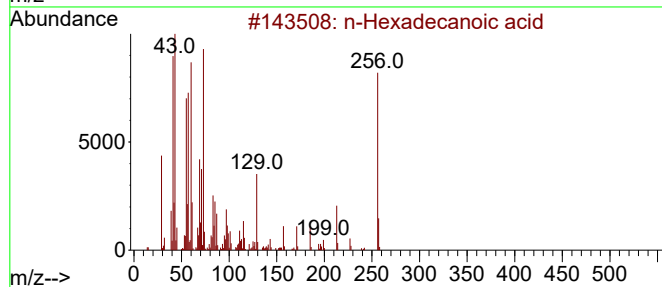
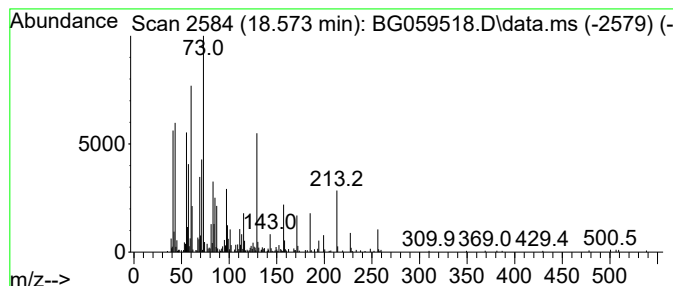
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.573	9.99 ng/ul	465596	Phenanthrene-d10	17.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059518.D
Acq On : 28 Oct 2023 12:26
Operator : MA/JU
Sample : 04925-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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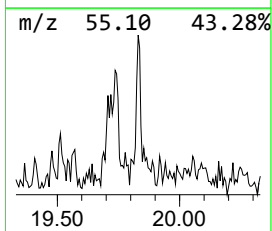
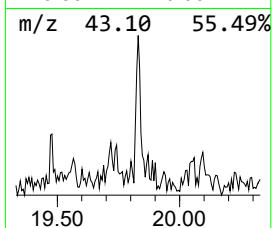
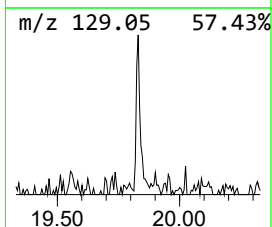
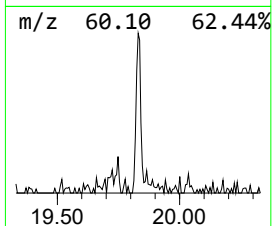
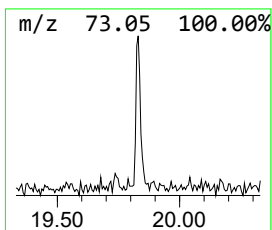
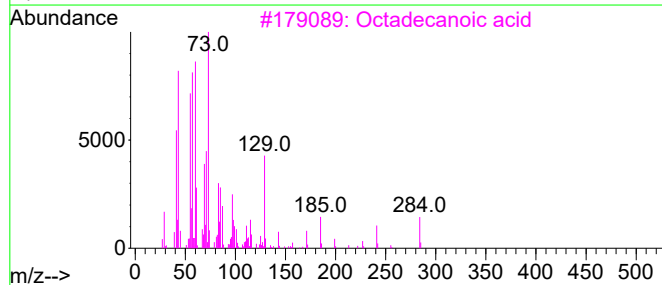
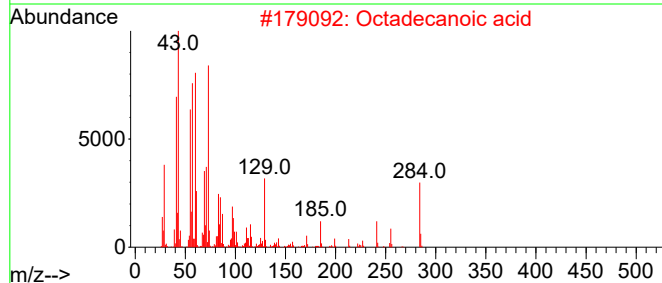
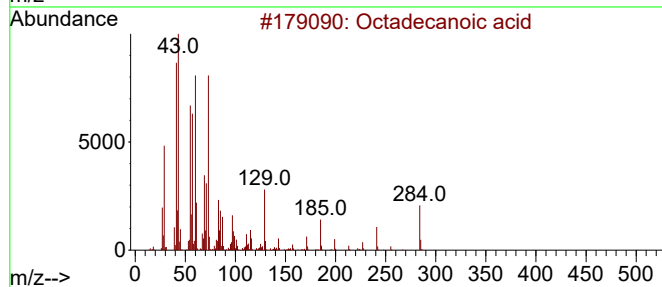
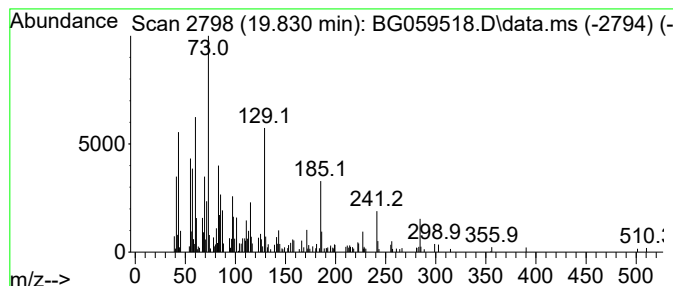
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.830	3.69 ng/ul	172089	Phenanthrene-d10	17.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	91
2			Octadecanoic acid	284	C18H36O2	000057-11-4	87
3			Octadecanoic acid	284	C18H36O2	000057-11-4	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059518.D
Acq On : 28 Oct 2023 12:26
Operator : MA/JU
Sample : 04925-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCW9

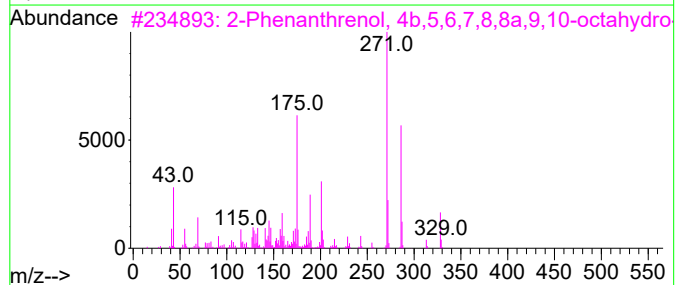
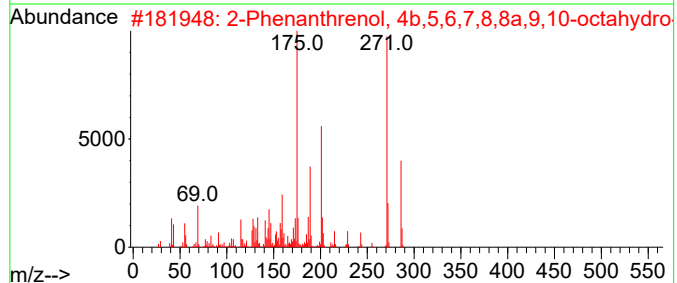
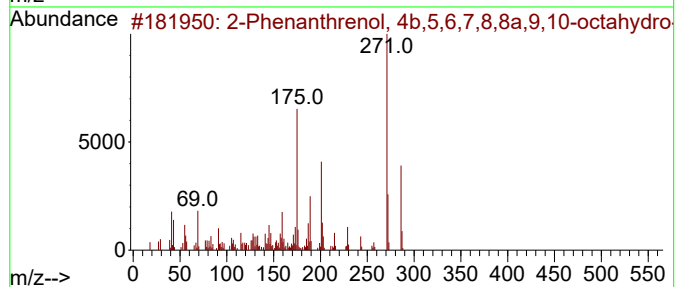
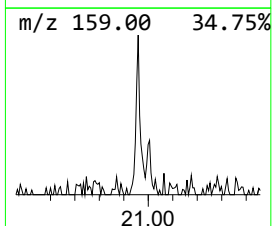
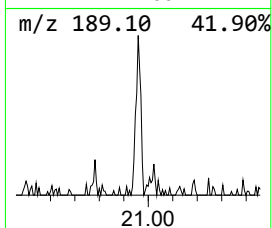
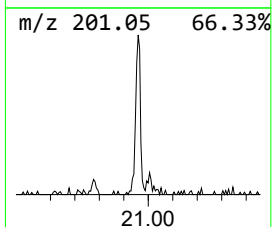
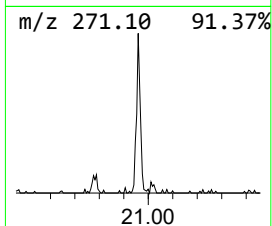
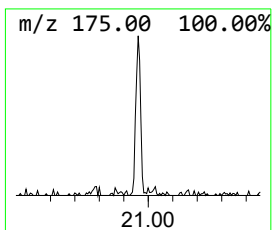
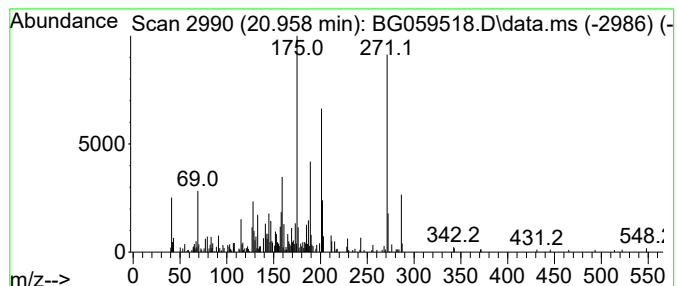
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.958	5.06 ng/ul	217489	Chrysene-d12	22.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	91
2			2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	45
3			2-Phenanthrenol, 4b,5,6,7,8,8a,9...	328	C22H32O2	015340-82-6	38
4			Propionic acid, 3,3,3-trifluoro...	330	C15H13F3O3S	1000276-91-1	35
5			Dipinacolyl dimethylpyrophosphonate	342	C14H32O5P2	081397-56-0	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059518.D
Acq On : 28 Oct 2023 12:26
Operator : MA/JU
Sample : 04925-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCW9

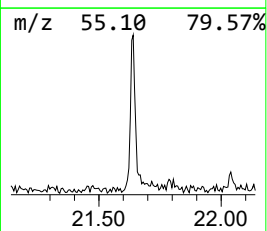
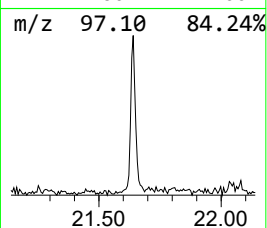
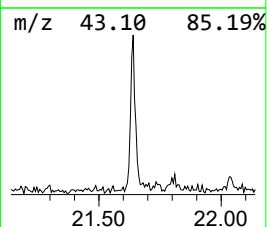
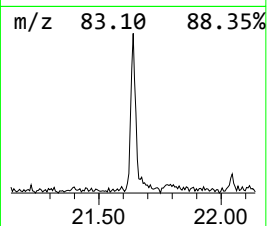
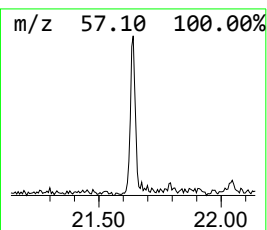
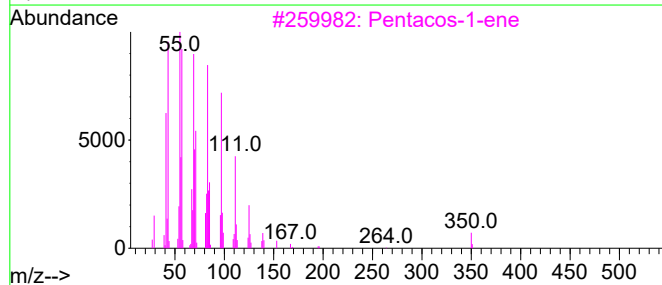
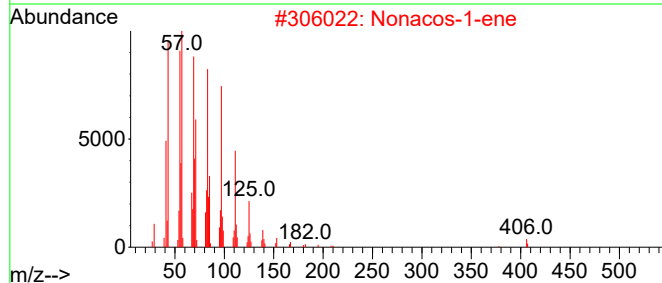
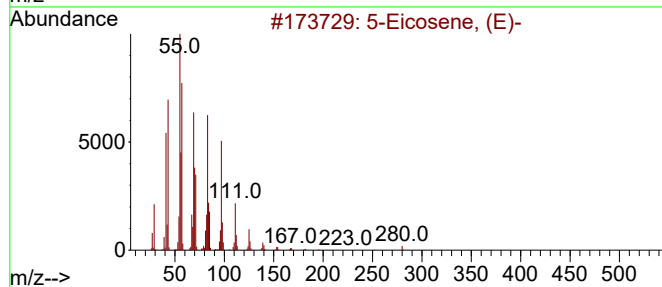
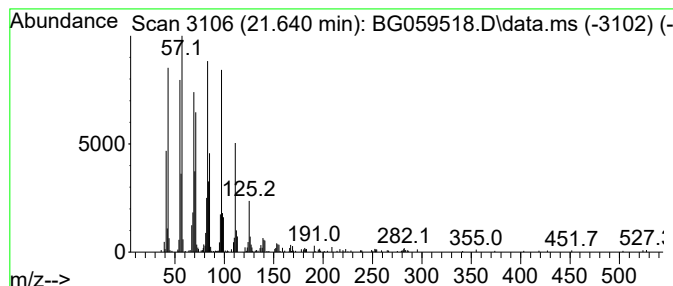
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.640	10.29 ng/ul	442350	Chrysene-d12	22.081

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
2	Nonacos-1-ene		406	C29H58	018835-35-3	90
3	Pentacos-1-ene		350	C25H50	016980-85-1	90
4	Heptacos-1-ene		378	C27H54	015306-27-1	90
5	1-Nonadecene		266	C19H38	018435-45-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG102823\
Data File : BG059518.D
Acq On : 28 Oct 2023 12:26
Operator : MA/JU
Sample : 04925-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GCCW9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\SFAM-EPA-BG102723.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
3-Pyridinol, 4-...	13.832	5.2	ng/ul	190917	3	14.995	735216	20.0
Juglone	15.248	5.8	ng/ul	214074	3	14.995	735216	20.0
9-Hexadecenoic ...	18.514	2.6	ng/ul	119449	4	17.744	931733	20.0
n-Hexadecanoic ...	18.573	10.0	ng/ul	465596	4	17.744	931733	20.0
Octadecanoic acid	19.830	3.7	ng/ul	172089	4	17.744	931733	20.0
2-Phenanthrenol...	20.958	5.1	ng/ul	217489	5	22.081	860170	20.0
(DEL) Alkane: S...	21.640	10.3	ng/ul	442350	5	22.081	860170	20.0