

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
 Data File : BP020674.D
 Acq On : 28 Jun 2024 00:32
 Operator : MA/JU
 Sample : P2909-04
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 A4B81

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-BP062524.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP020674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.011	3	4	18	rVB	1513283	1361194	40.78%	3.390%
2	3.275	45	49	56	rVB	29581	37366	1.12%	0.093%
3	3.546	92	95	104	rBV2	16479	27236	0.82%	0.068%
4	3.687	116	119	133	rBV	401736	556379	16.67%	1.386%
5	3.781	133	135	140	rVB4	7141	9124	0.27%	0.023%
6	4.005	168	173	178	rVB	12988	18024	0.54%	0.045%
7	4.552	263	266	271	rVB3	4890	7305	0.22%	0.018%
8	4.899	321	325	330	rBV2	16831	23336	0.70%	0.058%
9	5.152	363	368	371	rBV7	3835	6699	0.20%	0.017%
10	5.481	422	424	429	rVB6	4365	4717	0.14%	0.012%
11	5.864	484	489	495	rVB2	18889	30124	0.90%	0.075%
12	6.375	573	576	580	rVB5	2584	3530	0.11%	0.009%
13	6.781	640	645	646	rBV5	5153	6325	0.19%	0.016%
14	6.928	663	670	683	rVB	487804	749794	22.46%	1.867%
15	7.093	692	698	711	rVB	343590	552263	16.54%	1.375%
16	7.287	722	731	742	rBV	492092	777844	23.30%	1.937%
17	7.369	742	745	749	rBV4	5146	7959	0.24%	0.020%
18	7.746	802	809	817	rBV	507247	862761	25.84%	2.149%
19	7.816	817	821	829	rVB4	11485	21950	0.66%	0.055%
20	8.146	870	877	880	rBV8	3072	6664	0.20%	0.017%
21	8.446	920	928	941	rBV	592005	925919	27.74%	2.306%
22	8.852	990	997	998	rBV7	2577	5327	0.16%	0.013%
23	8.899	998	1005	1020	rVB	420217	723393	21.67%	1.802%
24	9.052	1029	1031	1035	rVB5	4954	5852	0.18%	0.015%
25	9.287	1067	1071	1075	rVB7	4305	5904	0.18%	0.015%
26	9.452	1093	1099	1109	rVB2	41655	73538	2.20%	0.183%
27	9.610	1119	1126	1134	rBV	330610	603097	18.07%	1.502%
28	9.834	1162	1164	1168	rBV5	3122	5046	0.15%	0.013%
29	10.146	1210	1217	1230	rBV	546517	944777	28.30%	2.353%
30	10.516	1272	1280	1291	rBV	640950	1154145	34.57%	2.874%
31	10.657	1291	1304	1321	rBV	393343	833656	24.97%	2.076%
32	11.057	1365	1372	1379	rBV9	10807	26472	0.79%	0.066%
33	11.257	1399	1406	1414	rVV	48951	103516	3.10%	0.258%
34	11.316	1414	1416	1423	rVB7	5838	8465	0.25%	0.021%
35	11.469	1435	1442	1446	rBV9	1480	3540	0.11%	0.009%
36	12.116	1545	1552	1557	rBV2	9528	15612	0.47%	0.039%

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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 >
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37	12.528	1618	1622	1627	rVB8	1829	3405	0.10%	0.008%
38	12.969	1694	1697	1703	rBV8	2628	4422	0.13%	0.011%
39	13.193	1727	1735	1740	rBV10	4433	11110	0.33%	0.028%
40	13.334	1755	1759	1762	rVV6	3131	4598	0.14%	0.011%
41	13.557	1791	1797	1800	rBV7	3665	5817	0.17%	0.014%
42	13.787	1829	1836	1851	rVB	859700	1328162	39.79%	3.308%
43	14.069	1872	1884	1900	rBV	1175728	1685146	50.48%	4.197%
44	14.281	1917	1920	1925	rVB6	3127	4788	0.14%	0.012%
45	14.381	1930	1937	1944	rBV	1039567	1452077	43.50%	3.616%
46	14.445	1944	1948	1953	rVV4	12013	20093	0.60%	0.050%
47	14.604	1967	1975	1989	rBV	311684	676377	20.26%	1.684%
48	14.751	1996	2000	2003	rBV5	5154	8697	0.26%	0.022%
49	14.810	2003	2010	2017	rVB9	11513	30566	0.92%	0.076%
50	15.181	2070	2073	2075	rBV4	2951	4149	0.12%	0.010%
51	15.251	2082	2085	2091	rBV7	3859	6443	0.19%	0.016%
52	15.392	2102	2109	2116	rBV	1367949	2044112	61.23%	5.091%
53	15.451	2116	2119	2124	rVB3	11572	15705	0.47%	0.039%
54	15.516	2124	2130	2144	rBV	308487	536151	16.06%	1.335%
55	15.828	2179	2183	2188	rBV8	4242	8124	0.24%	0.020%
56	15.904	2191	2196	2202	rBV10	4115	11272	0.34%	0.028%
57	16.139	2232	2236	2242	rVB6	8666	12770	0.38%	0.032%
58	16.316	2257	2266	2271	rBV6	13138	41723	1.25%	0.104%
59	16.586	2308	2312	2314	rBV5	14255	21669	0.65%	0.054%
60	17.186	2408	2414	2419	rBV	1128833	1748784	52.39%	4.355%
61	17.228	2419	2421	2426	rVV	122695	167021	5.00%	0.416%
62	17.298	2426	2433	2443	rVV	1345570	2194237	65.73%	5.464%
63	17.610	2484	2486	2490	rBV	13448	13463	0.40%	0.034%
64	18.128	2569	2574	2585	rVB2	321502	474384	14.21%	1.181%
65	18.310	2600	2605	2608	rBV2	21662	38028	1.14%	0.095%
66	18.792	2684	2687	2689	rBV4	25346	34380	1.03%	0.086%
67	18.828	2690	2693	2697	rVV5	56306	89504	2.68%	0.223%
68	19.227	2758	2761	2764	rBV4	47408	49083	1.47%	0.122%
69	19.328	2774	2778	2790	rVB	367831	585399	17.54%	1.458%
70	19.475	2795	2803	2807	rBV2	187019	366210	10.97%	0.912%
71	19.675	2831	2837	2848	rVB3	1941307	3338254	100.00%	8.313%
72	19.863	2863	2869	2871	rBV6	108163	193106	5.78%	0.481%
73	19.904	2871	2876	2879	rVV2	308920	397312	11.90%	0.989%
74	19.980	2887	2889	2896	rVB6	81415	121057	3.63%	0.301%
75	20.180	2919	2923	2925	rBV5	110818	168404	5.04%	0.419%
76	20.204	2925	2927	2930	rVV3	89438	109678	3.29%	0.273%

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77	20.322	2945	2947	2948	rBV	114574	93848	2.81%	0.234%
78	20.592	2990	2993	2994	rBV3	76352	82784	2.48%	0.206%
79	20.633	2995	3000	3001	rVV5	277943	439668	13.17%	1.095%
80	20.651	3001	3003	3009	rVB	394974	498192	14.92%	1.241%
81	20.922	3045	3049	3051	rBV5	139390	229214	6.87%	0.571%
82	21.316	3112	3116	3123	rBV3	362847	576635	17.27%	1.436%
83	21.380	3125	3127	3128	rBV2	106626	96159	2.88%	0.239%
84	21.404	3128	3131	3136	rVB3	217491	386991	11.59%	0.964%
85	21.651	3166	3173	3178	rBV2	1304323	2466921	73.90%	6.144%
86	22.821	3370	3372	3381	rVB9	211728	422211	12.65%	1.051%
87	23.551	3494	3496	3498	rBV2	185771	163209	4.89%	0.406%
88	24.792	3697	3707	3714	rVB	1155401	2940053	88.07%	7.322%
89	25.021	3739	3746	3763	rVB	966027	3099135	92.84%	7.718%
90	25.933	3899	3901	3904	rBV4	99141	125119	3.75%	0.312%

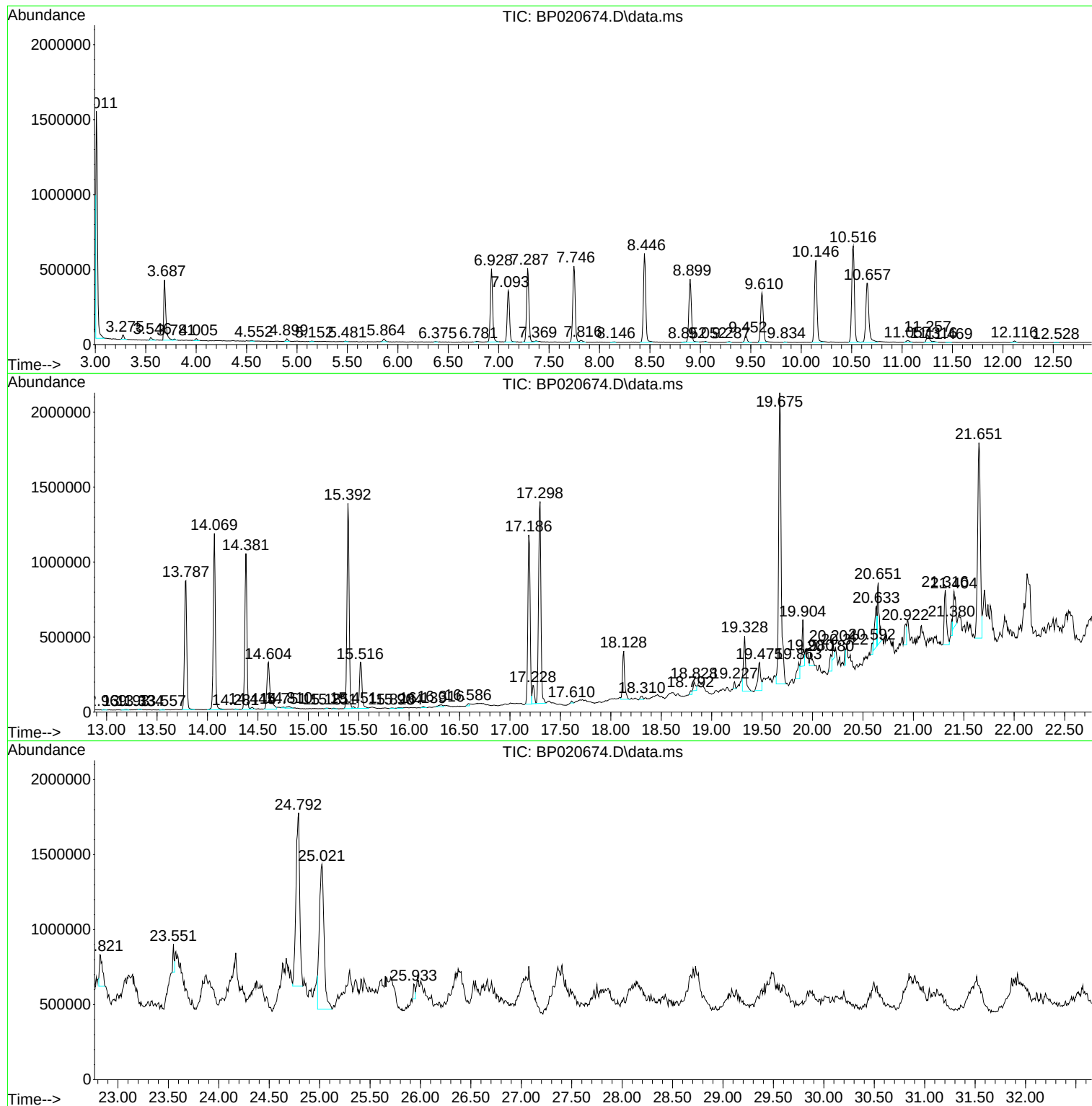
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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



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Instrument :
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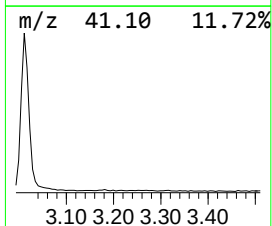
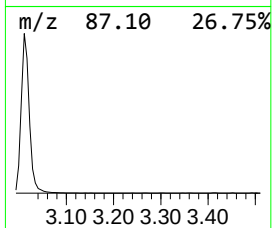
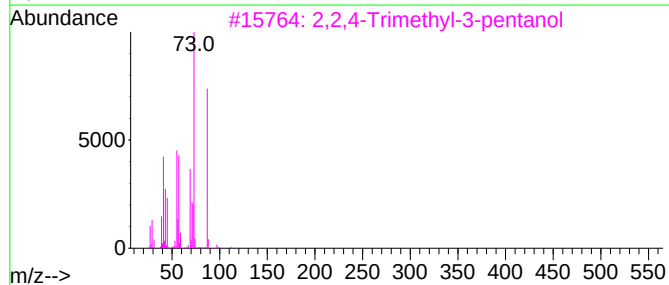
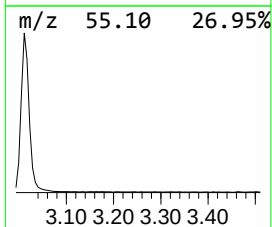
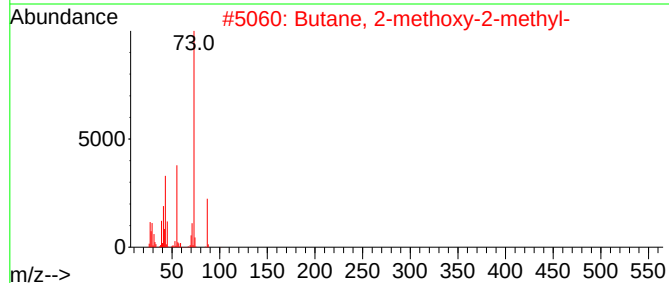
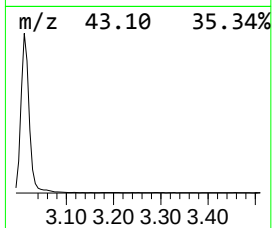
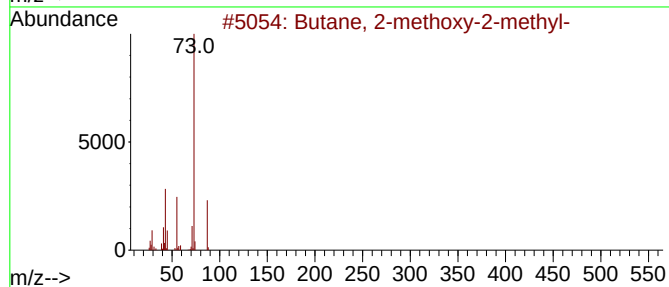
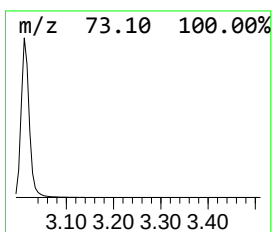
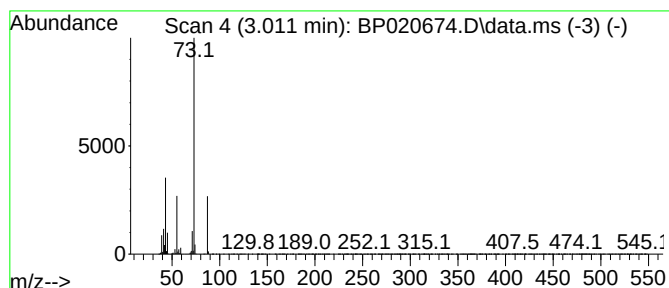
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.011	31.55 ng/ul	1361190	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78		
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64		
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40		
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17		
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9		



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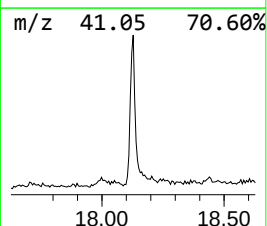
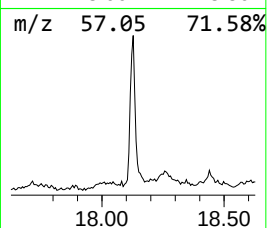
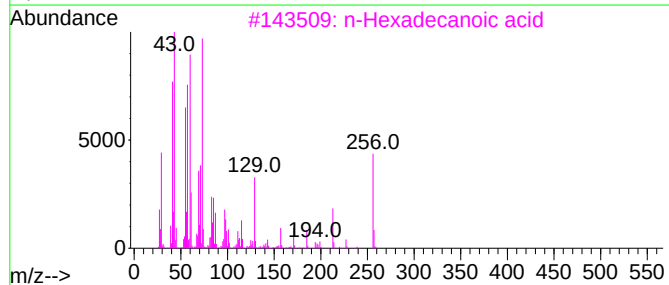
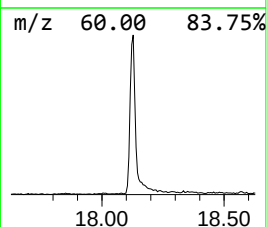
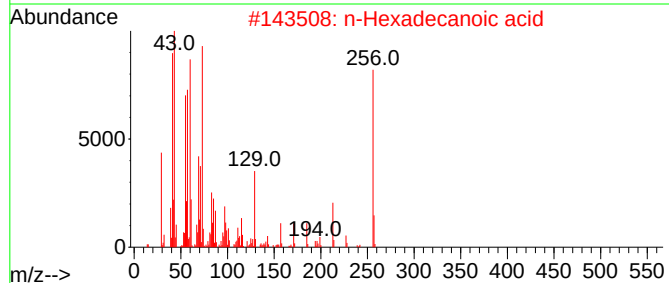
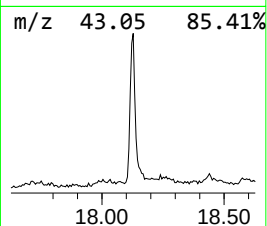
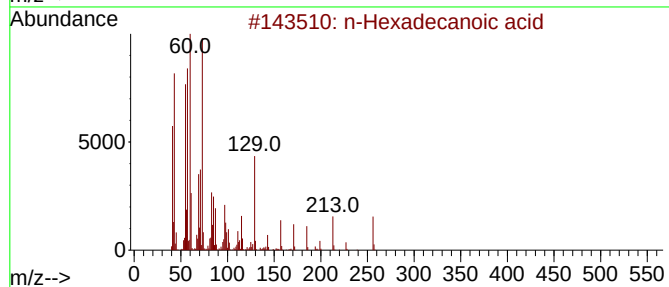
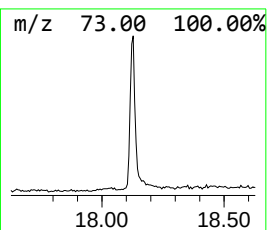
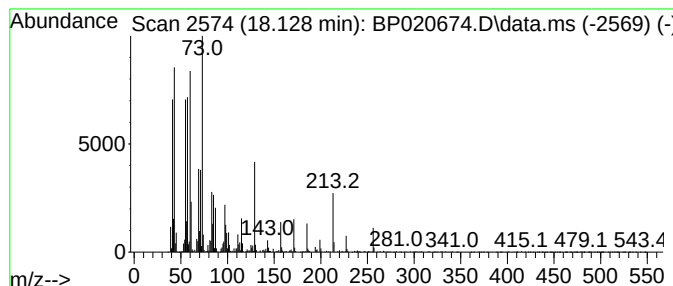
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.128	5.43 ng/ul	474384	Phenanthrene-d10	17.186

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	97		
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93		



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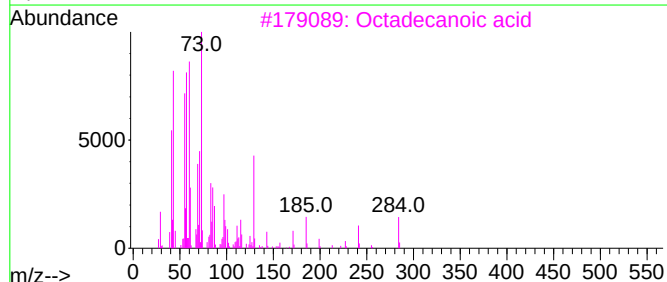
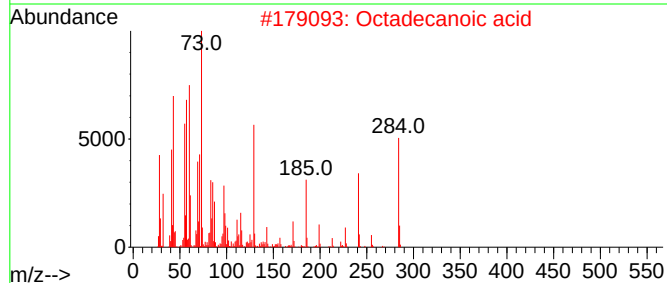
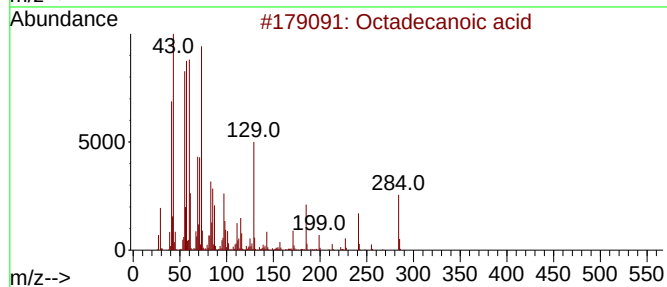
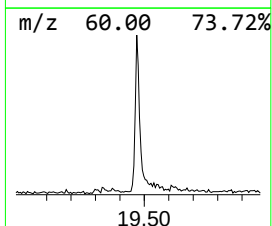
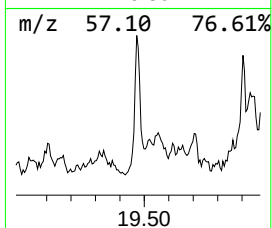
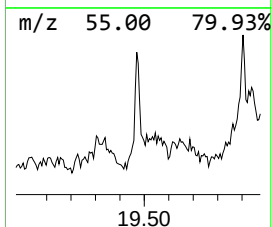
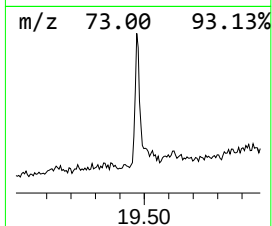
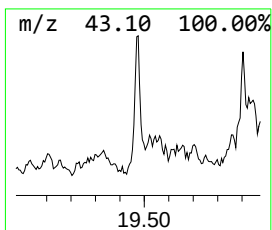
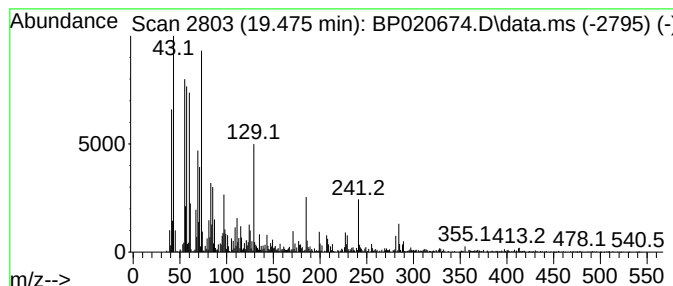
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.475	2.97 ng/ul	366210	Chrysene-d12	21.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid	284	C18H36O2	000057-11-4	98
3			Octadecanoic acid	284	C18H36O2	000057-11-4	96
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90



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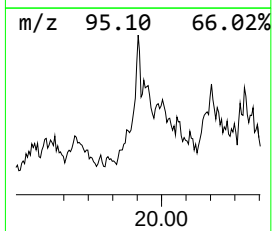
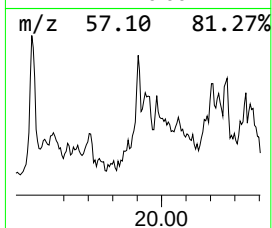
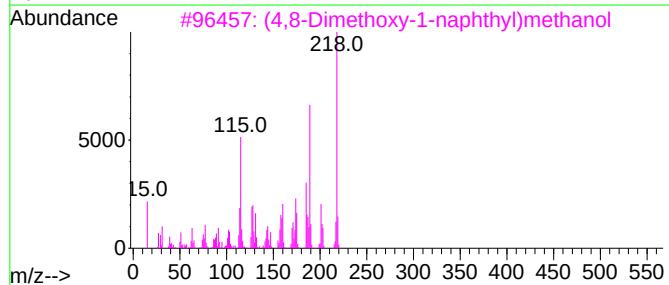
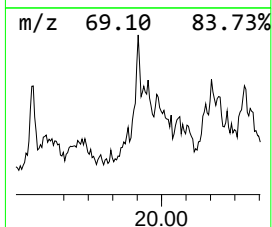
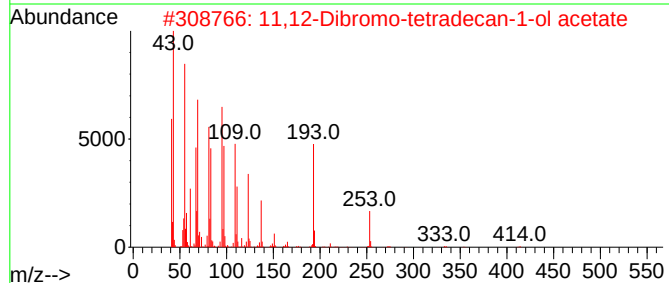
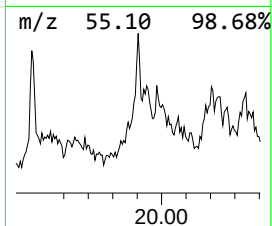
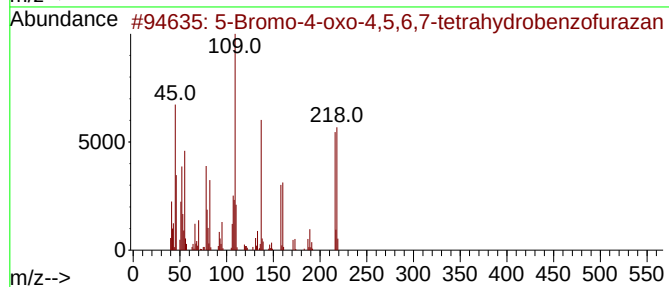
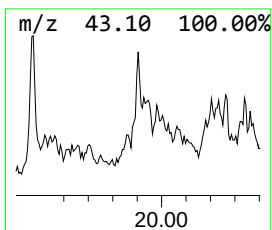
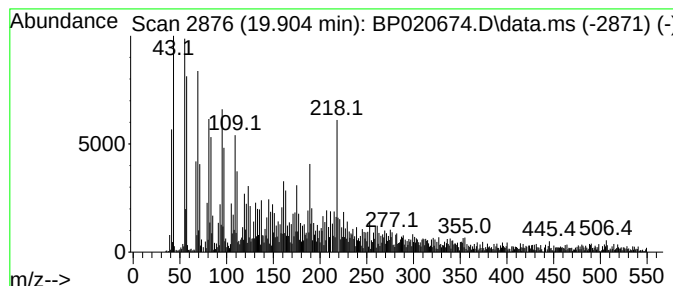
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.904	3.22 ng/ul	397312	Chrysene-d12	21.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	83
2			11,12-Dibromo-tetradecan-1-ol ac...	412	C16H30Br2O2	1000130-78-5	50
3			(4,8-Dimethoxy-1-naphthyl)methanol	218	C13H14O3	1000460-12-1	48
4			D-Homoandrostande, (5.alpha.,13.a...	274	C20H34	054482-31-4	46
5			30-Norlupan-28-oic acid, 3-hydro...	502	C31H50O5	055401-91-7	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
Data File : BP020674.D
Acq On : 28 Jun 2024 00:32
Operator : MA/JU
Sample : P2909-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4B81

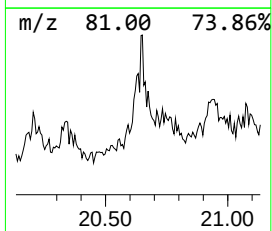
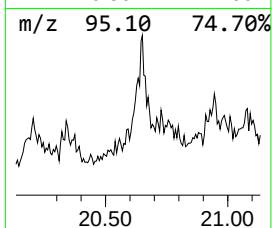
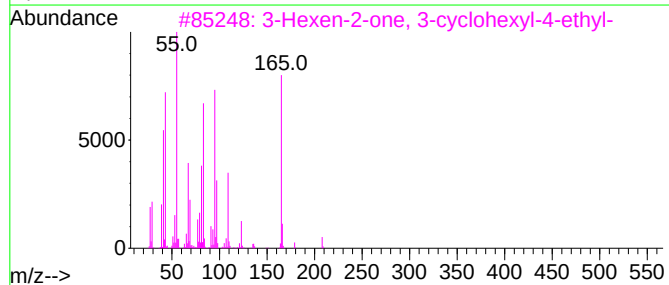
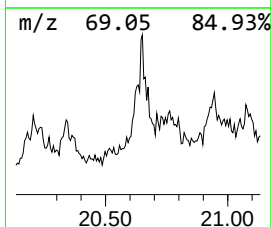
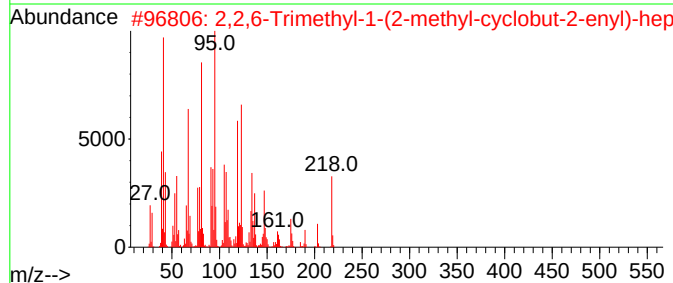
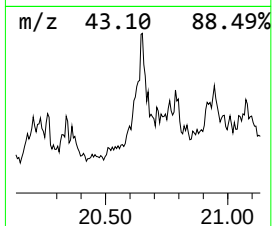
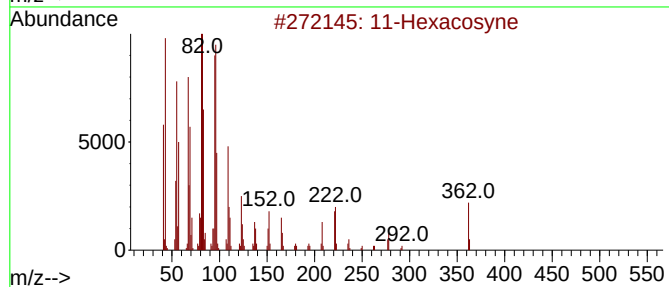
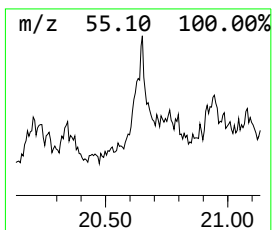
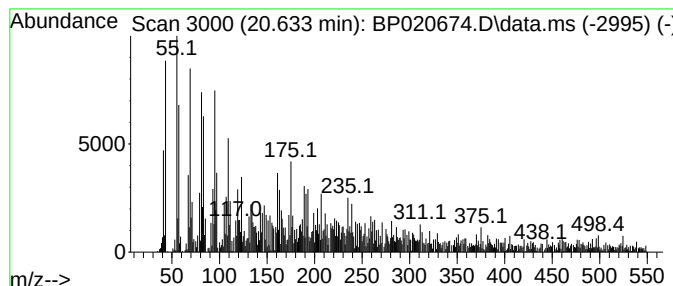
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 11-Hexacosyne Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.633	3.56 ng/ul	439668	Chrysene-d12	21.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Hexacosyne	362	C26H50	034291-69-5	70
2			2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	70
3			3-Hexen-2-one, 3-cyclohexyl-4-et...	208	C14H24O	1000150-19-1	55
4			Methyl 2-octylcyclopropene-1-hep...	294	C19H34O2	005026-66-4	55
5			5.alpha.-Cholest-22-ene, (Z)-	370	C27H46	015076-93-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
Data File : BP020674.D
Acq On : 28 Jun 2024 00:32
Operator : MA/JU
Sample : P2909-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

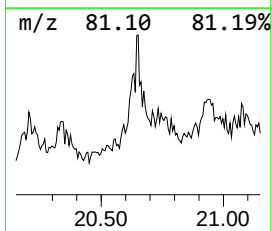
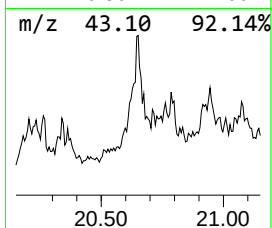
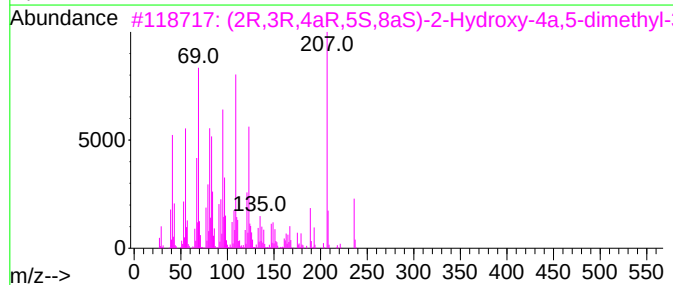
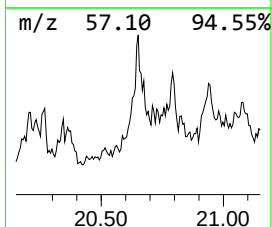
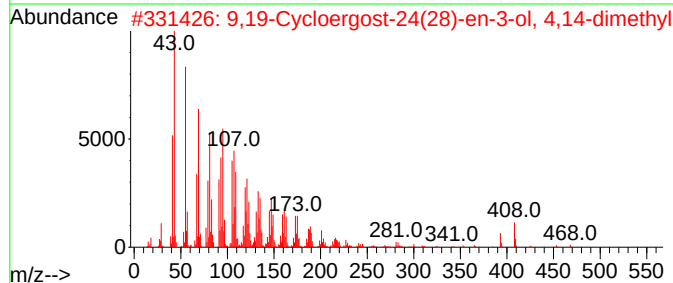
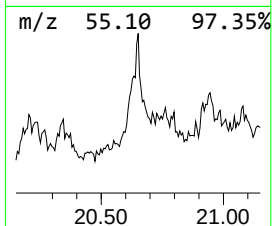
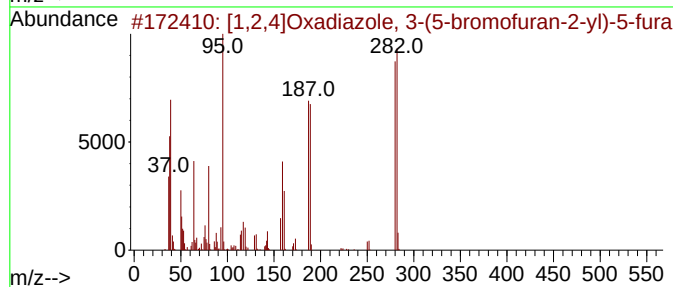
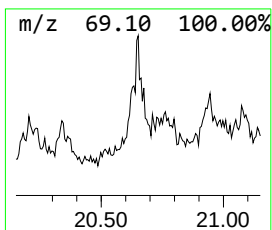
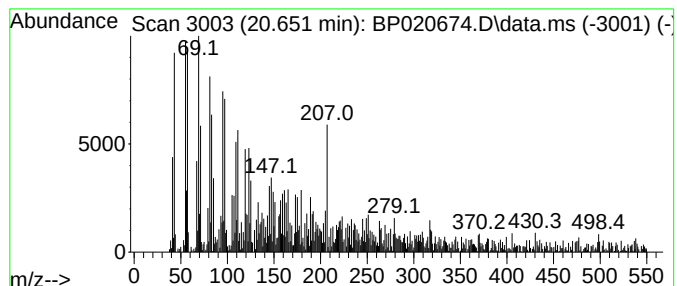
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ClientSampleId :
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 [1,2,4]Oxadiazole, 3-(5-bro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.651	4.04 ng/ul	498192	Chrysene-d12	21.651	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[1,2,4]Oxadiazole, 3-(5-bromofur...	280	C10H5BrN2O3	1000303-56-3	91
2	9,19-Cycloergost-24(28)-en-3-ol,...	468	C32H52O2	010376-42-8	78
3	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,...	236	C15H24O2	066884-74-0	60
4	2a,5,5,10b-Tetramethyl-3,4,4a,5,...	285	C18H23NO2	1000274-52-8	60
5	Furane-2-carboxamide, N-propyl-N...	405	C26H47NO2	1000437-96-7	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
Data File : BP020674.D
Acq On : 28 Jun 2024 00:32
Operator : MA/JU
Sample : P2909-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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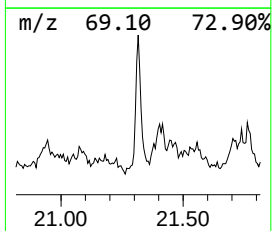
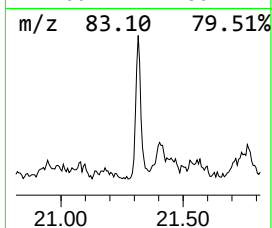
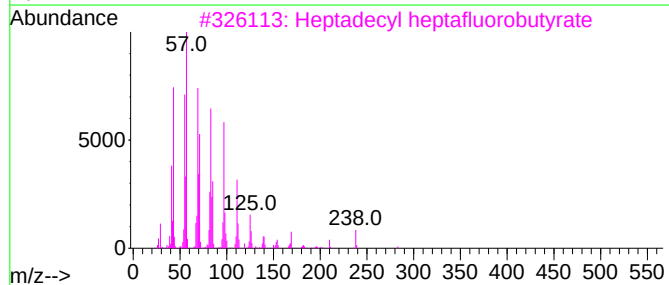
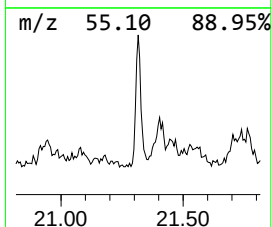
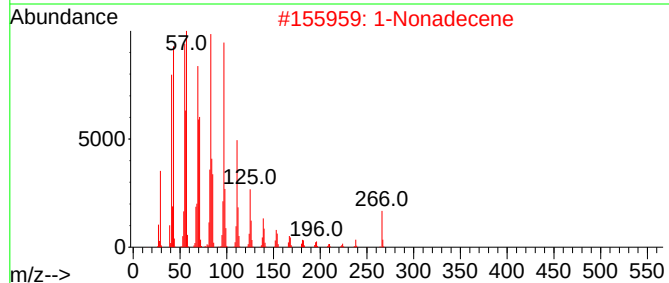
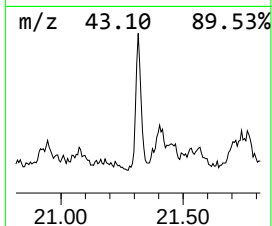
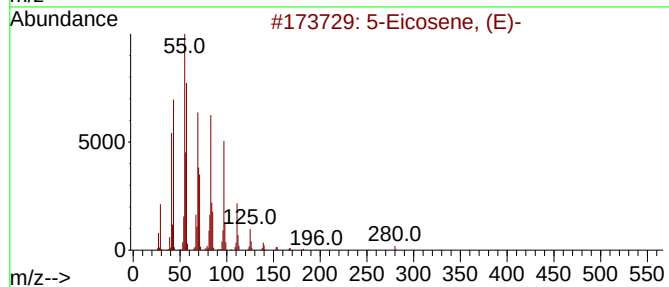
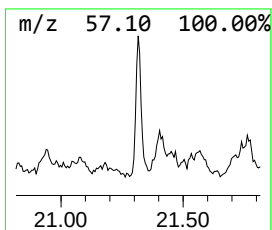
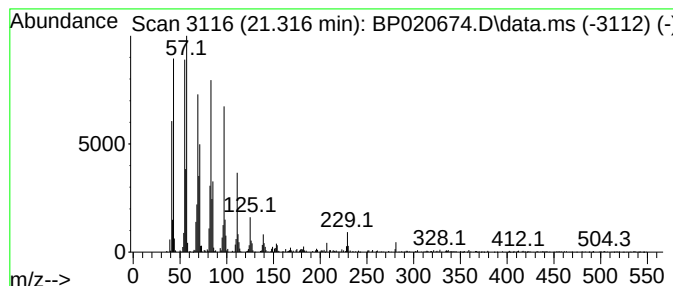
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Quant Title : SVOA CALIBRATION

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.316	4.67 ng/ul	576635	Chrysene-d12	21.651

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	1-Nonadecene		266	C19H38	018435-45-5	96
3	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
4	1-Hexacosene		364	C26H52	018835-33-1	94
5	Pentacos-1-ene		350	C25H50	016980-85-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
Data File : BP020674.D
Acq On : 28 Jun 2024 00:32
Operator : MA/JU
Sample : P2909-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
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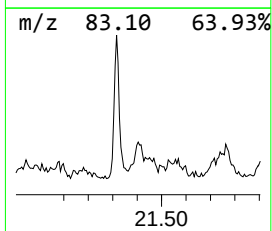
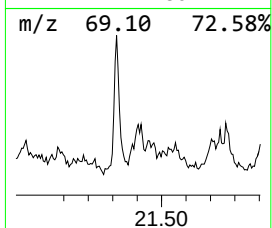
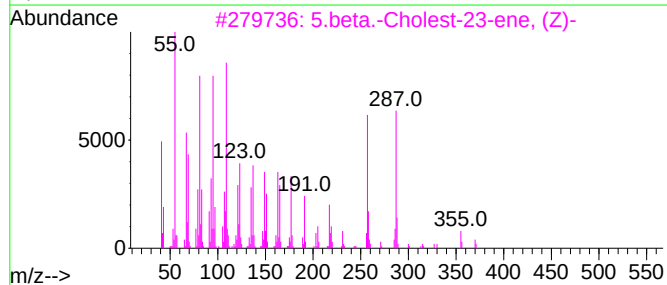
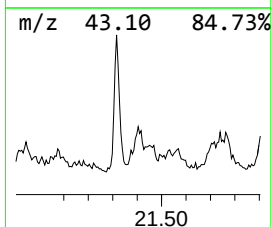
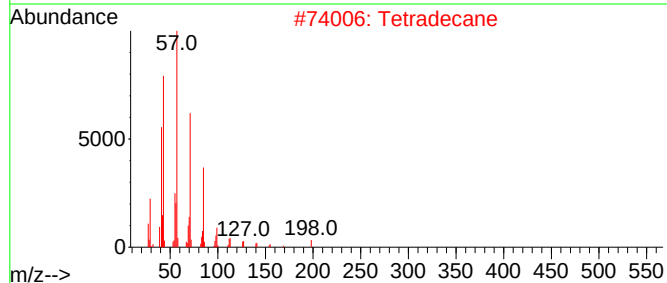
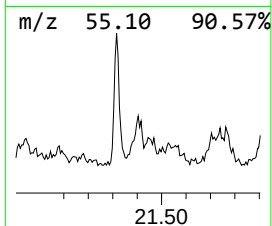
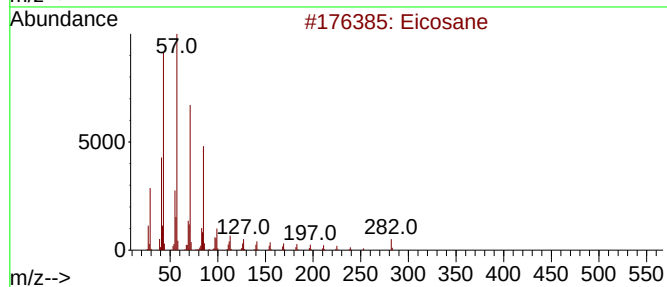
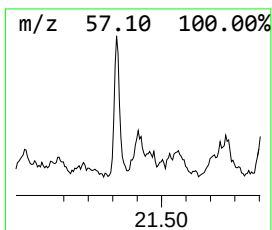
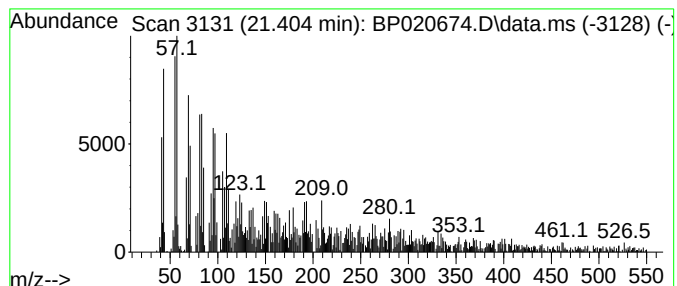
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.404	3.14 ng/ul	386991	Chrysene-d12	21.651

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	90
2			Tetradecane	198	C14H30	000629-59-4	90
3			5.beta.-Cholest-23-ene, (Z)-	370	C27H46	014949-12-3	86
4			Fumaric acid, 4-chlorophenyl dod...	394	C22H31ClO4	1000344-86-1	66
5			2,5-Furandione, dihydro-3-octade...	352	C22H40O3	047458-32-2	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062724\
Data File : BP020674.D
Acq On : 28 Jun 2024 00:32
Operator : MA/JU
Sample : P2909-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062524.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
Butane, 2-metho...	3.011	31.6	ng/ul	1361190	1	7.746	862761	20.0
n-Hexadecanoic ...	18.128	5.4	ng/ul	474384	4	17.186	1748780	20.0
Octadecanoic acid	19.475	3.0	ng/ul	366210	5	21.651	2466920	20.0
5-Bromo-4-oxo-4...	19.904	3.2	ng/ul	397312	5	21.651	2466920	20.0
11-Hexacosyne	20.633	3.6	ng/ul	439668	5	21.651	2466920	20.0
[1,2,4]Oxadiaz...	20.651	4.0	ng/ul	498192	5	21.651	2466920	20.0
(DEL) Alkane: S...	21.316	4.7	ng/ul	576635	5	21.651	2466920	20.0
(DEL) Alkane: S...	21.404	3.1	ng/ul	386991	5	21.651	2466920	20.0
1,1,6-trimethyl...	22.821	3.4	ng/ul	422211	5	21.651	2466920	20.0