

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
 Data File : BP015695.D
 Acq On : 24 Jun 2023 05:02
 Operator : MA/JU
 Sample : 03085-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFP0

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-BP060723.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.399	33	36	43	rVB	33440	41939	0.25%	0.077%
2	3.870	115	116	126	rVV	22484	47107	0.28%	0.086%
3	3.946	126	129	137	rVV	45748	67607	0.40%	0.124%
4	4.070	145	150	155	rVB	20841	33476	0.20%	0.061%
5	4.170	163	167	172	rVB	14613	20551	0.12%	0.038%
6	7.246	684	690	710	rBV	304115	628396	3.67%	1.152%
7	7.399	710	716	727	rBV	325519	558868	3.27%	1.024%
8	7.605	745	751	768	rBV	419104	742589	4.34%	1.361%
9	8.075	823	831	845	rBV	536323	946573	5.53%	1.735%
10	8.811	947	956	970	rBV	152463	345453	2.02%	0.633%
11	9.263	1026	1033	1054	rBV	367078	720955	4.21%	1.321%
12	9.993	1148	1157	1174	rBV	292227	603340	3.53%	1.106%
13	10.546	1243	1251	1278	rBV	241258	714647	4.18%	1.310%
14	10.905	1304	1312	1325	rBV	634829	1126925	6.59%	2.065%
15	11.075	1333	1341	1368	rBV	105062	368172	2.15%	0.675%
16	14.134	1852	1861	1876	rVV	705685	1090017	6.37%	1.997%
17	14.422	1903	1910	1925	rBV	830025	1298709	7.59%	2.380%
18	14.728	1955	1962	1972	rBV	791238	1217691	7.12%	2.231%
19	15.016	2003	2011	2019	rBV4	27595	92782	0.54%	0.170%
20	15.722	2125	2131	2149	rBV	933266	1522539	8.90%	2.790%
21	15.881	2152	2158	2170	rBV3	91691	212597	1.24%	0.390%
22	16.093	2188	2194	2204	rBV	383633	636188	3.72%	1.166%
23	16.581	2273	2277	2280	rBV6	11895	18129	0.11%	0.033%
24	16.651	2284	2289	2299	rVB	104645	159997	0.93%	0.293%
25	17.016	2347	2351	2360	rVB3	17781	27147	0.16%	0.050%
26	17.369	2407	2411	2417	rBV5	17650	29054	0.17%	0.053%
27	17.487	2425	2431	2440	rVV	885307	1397756	8.17%	2.561%
28	17.592	2443	2449	2461	rVB	930091	1501299	8.77%	2.751%
29	18.234	2555	2558	2563	rVB6	13775	18232	0.11%	0.033%
30	18.292	2563	2568	2572	rBV	75906	110106	0.64%	0.202%
31	18.345	2572	2577	2586	rBV	513302	714193	4.17%	1.309%
32	18.622	2621	2624	2631	rBV5	18814	38670	0.23%	0.071%
33	19.228	2724	2727	2733	rVB5	24751	29383	0.17%	0.054%
34	19.434	2759	2762	2764	rBV3	51722	65297	0.38%	0.120%
35	19.463	2764	2767	2768	rBV3	39630	46243	0.27%	0.085%
36	19.569	2782	2785	2795	rBV2	136824	231506	1.35%	0.424%

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37	19.816	2822	2827	2840	rVB	1492591	2100805	12.28%	3.850%
38	21.251	3066	3071	3078	rBV	515009	809590	4.73%	1.484%
39	21.580	3122	3127	3137	rVB	1208150	1725571	10.08%	3.162%
40	22.169	3225	3227	3230	rVV	126715	130123	0.76%	0.238%
41	22.210	3231	3234	3241	rVB	206605	333420	1.95%	0.611%
42	23.286	3413	3417	3424	rVB	544420	847575	4.95%	1.553%
43	23.969	3527	3533	3546	rVB2	1157765	2503093	14.63%	4.587%
44	24.139	3556	3562	3572	rVB	841251	1866313	10.91%	3.420%
45	24.739	3658	3664	3675	rVB	992369	2171735	12.69%	3.980%
46	24.869	3683	3686	3699	rVB2	334641	835097	4.88%	1.530%
47	26.727	3995	4002	4020	rVB2	882153	3302281	19.30%	6.051%
48	27.815	4179	4187	4207	rVB3	830222	3407584	19.91%	6.244%
49	28.886	4358	4369	4388	rVB3	4099746	17113302	100.00%	31.360%

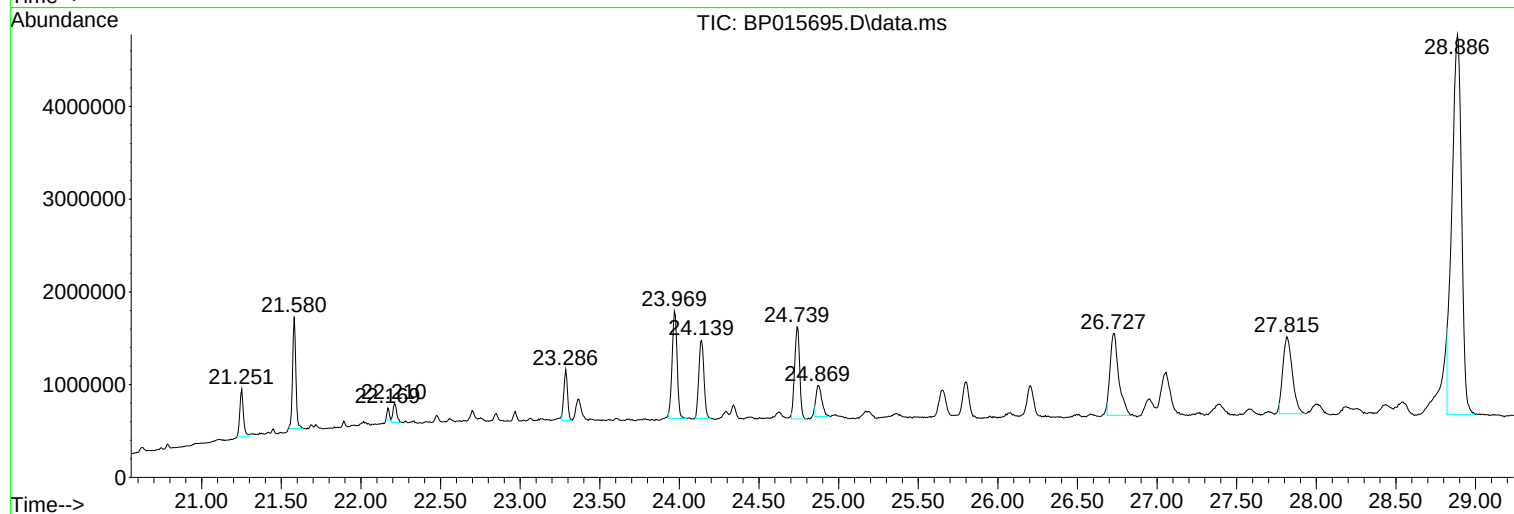
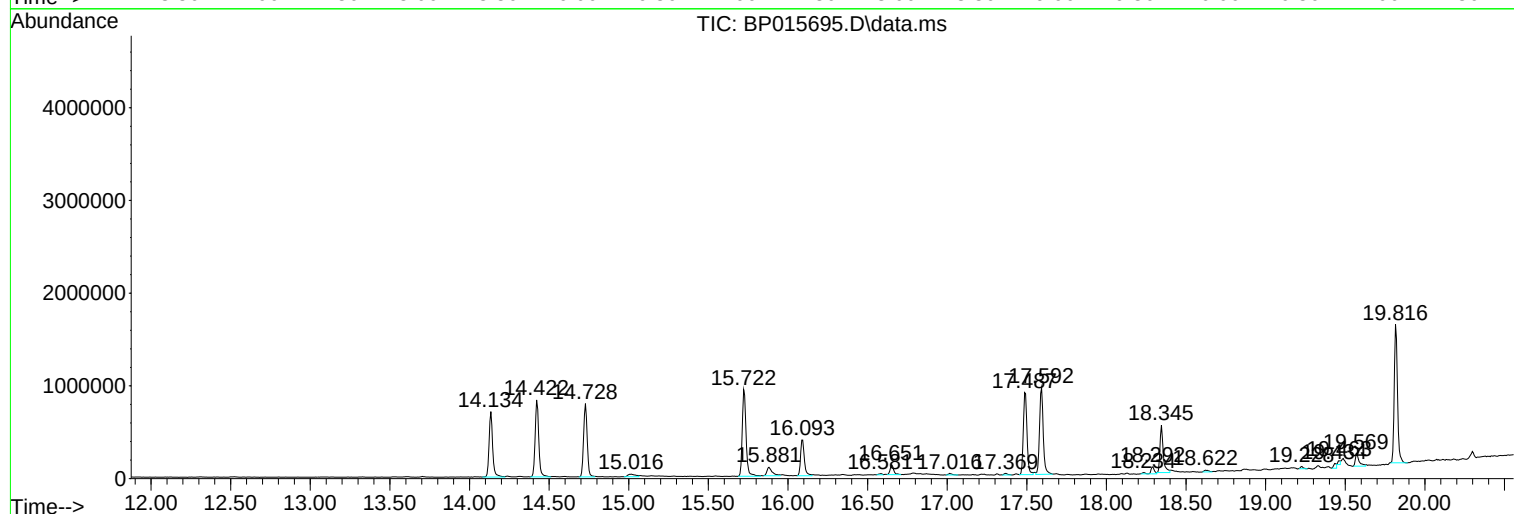
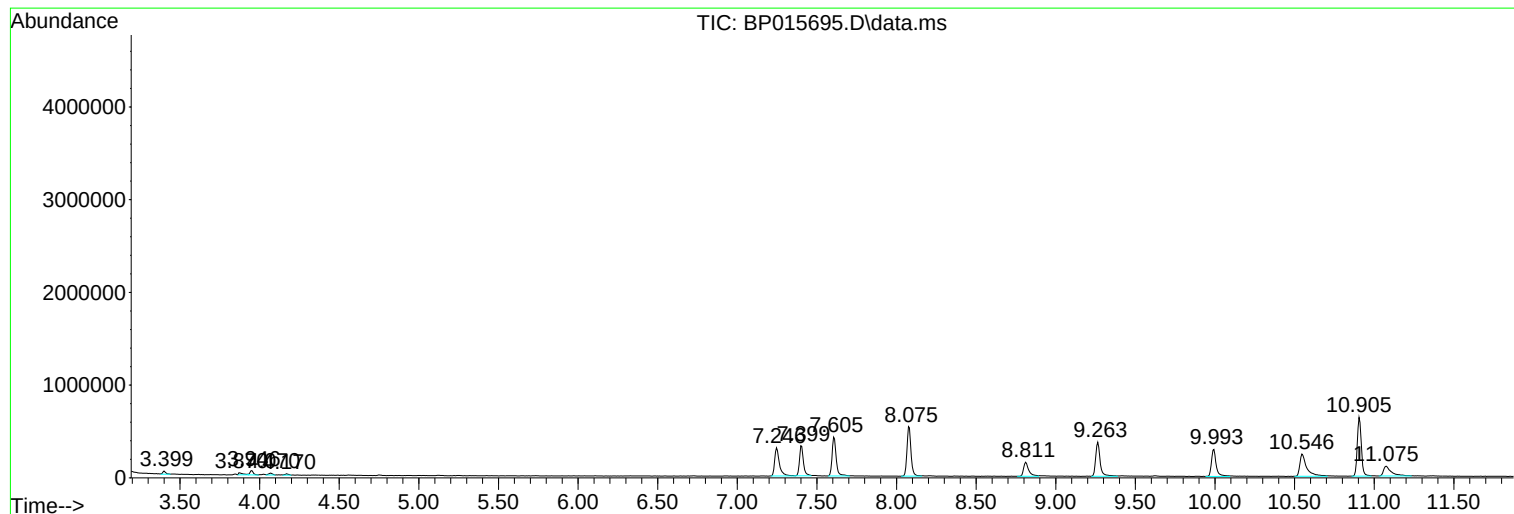
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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



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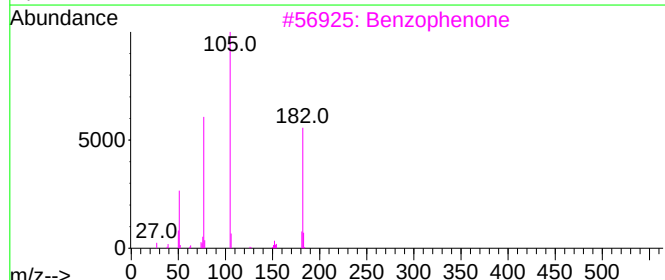
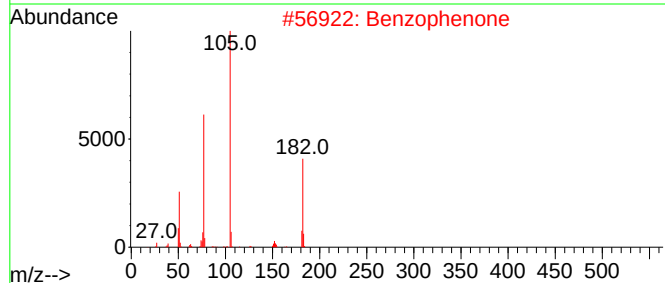
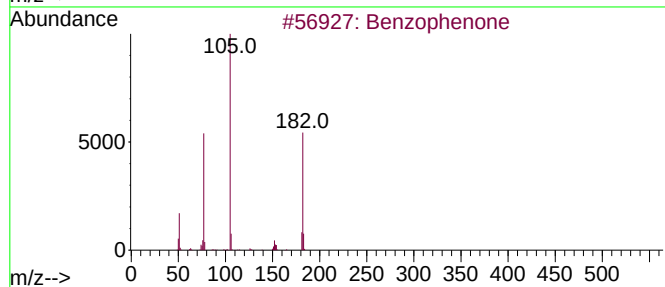
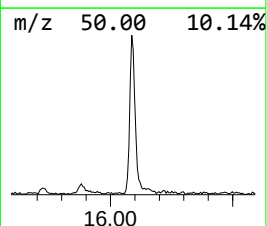
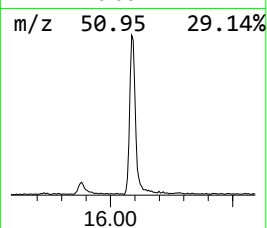
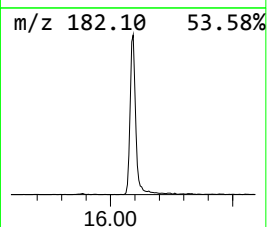
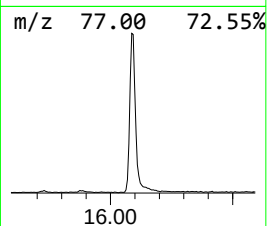
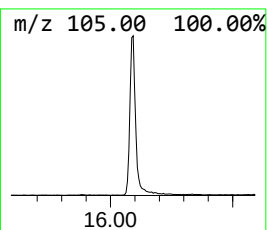
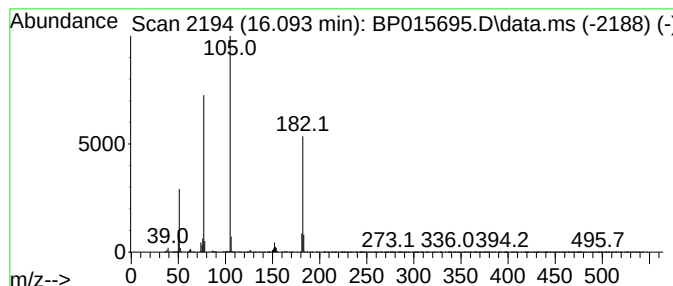
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.093	10.45 ng/ul	636188	Acenaphthene-d10	14.728

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzophenone	182	C13H10O	000119-61-9	96
3			Benzophenone	182	C13H10O	000119-61-9	96
4			Benzophenone	182	C13H10O	000119-61-9	95
5			Benzophenone	182	C13H10O	000119-61-9	91



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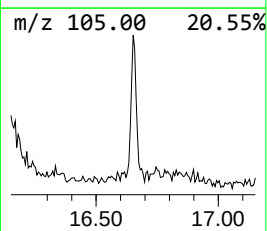
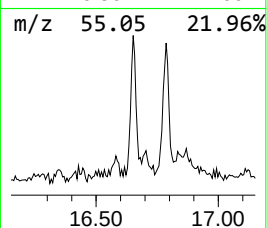
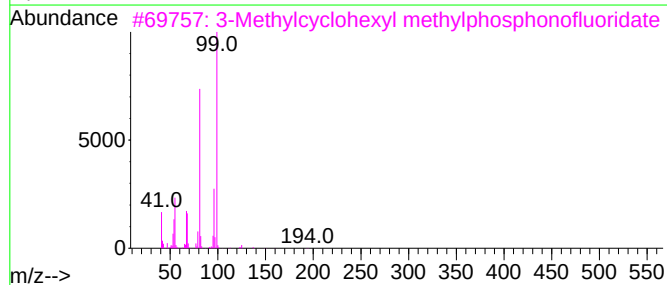
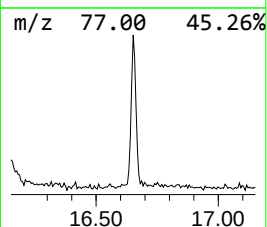
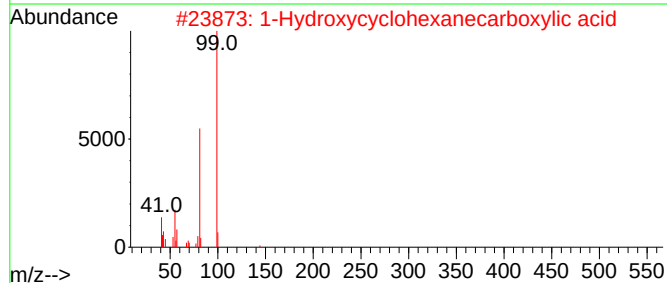
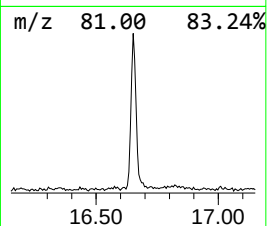
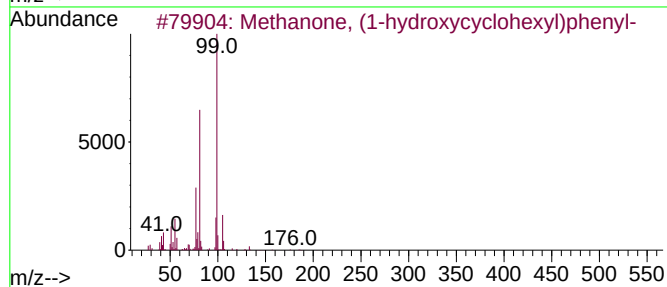
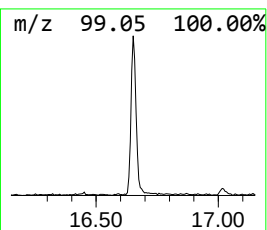
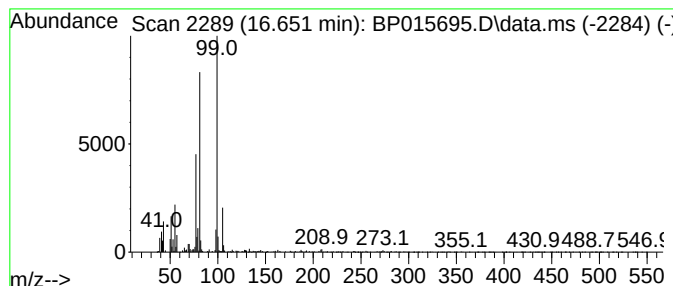
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 Methanone, (1-hydroxycyclohexyl) Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.651	2.29 ng/ul	159997	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	80
2			1-Hydroxycyclohexanecarboxylic acid	144	C7H12O3	001123-28-0	50
3			3-Methylcyclohexyl methylphospho...	194	C8H16FO2P	113548-86-0	50
4			Methanone, (1-hydroxycyclohexyl)...	204	C13H16O2	000947-19-3	49
5			Cyclohexanol, 1-(aminomethyl)-	129	C7H15NO	004000-72-0	43



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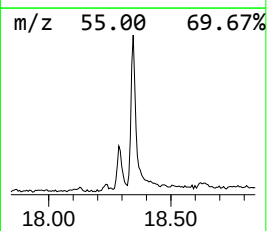
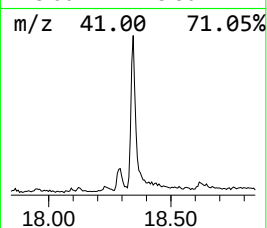
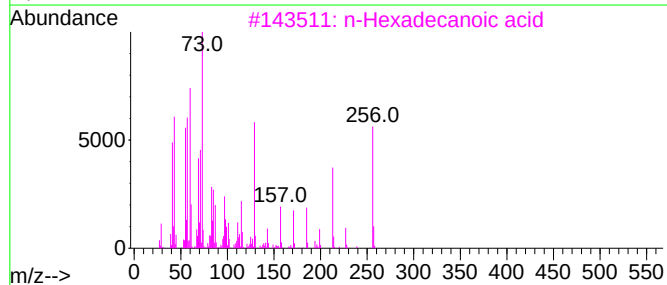
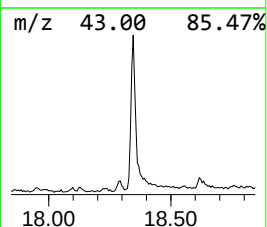
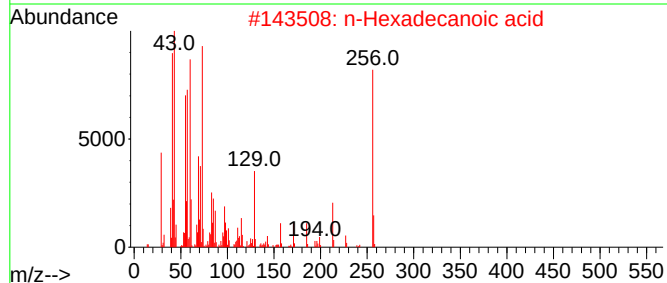
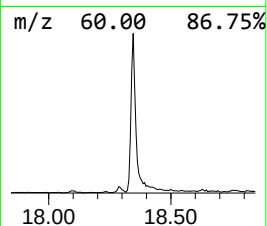
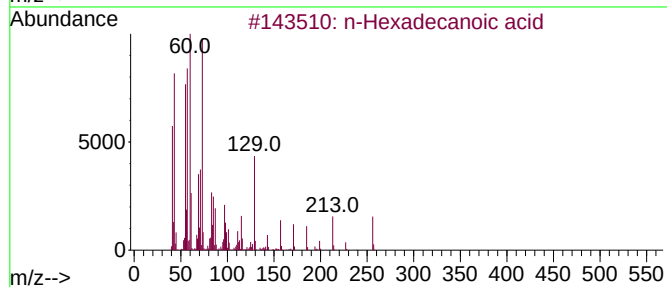
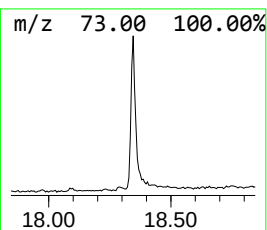
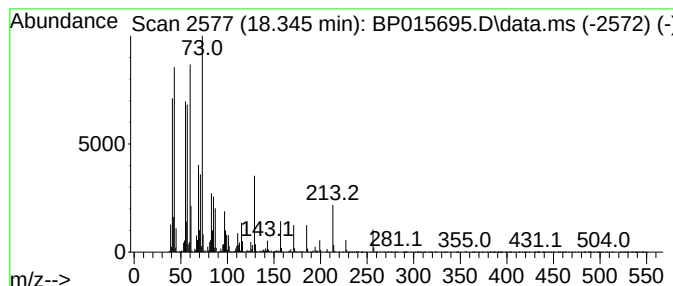
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.345	10.22 ng/ul	714193	Phenanthrene-d10	17.487

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	97
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



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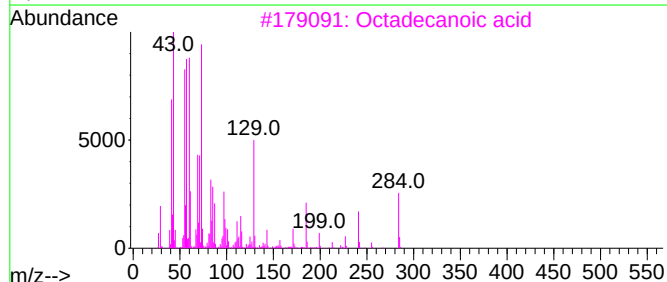
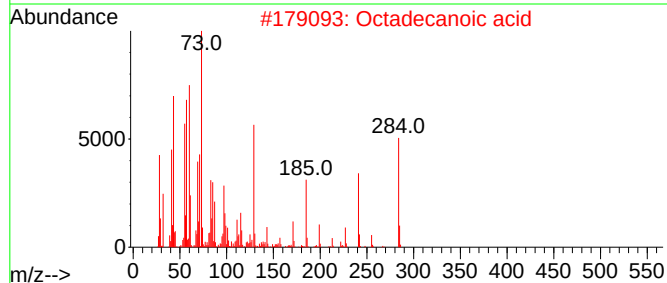
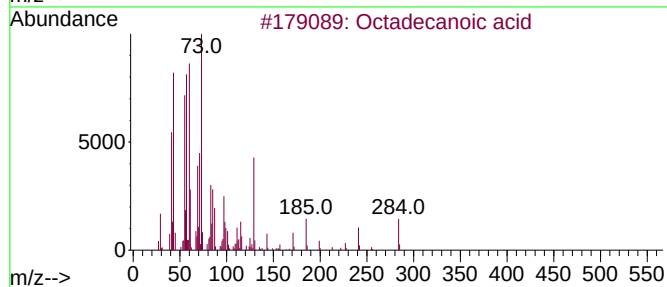
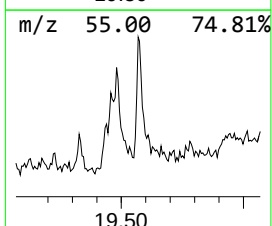
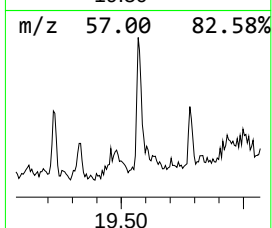
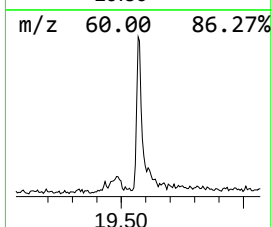
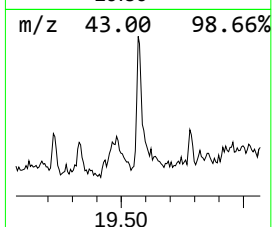
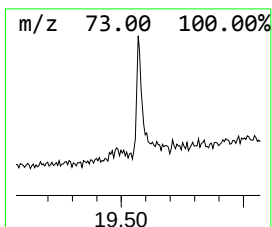
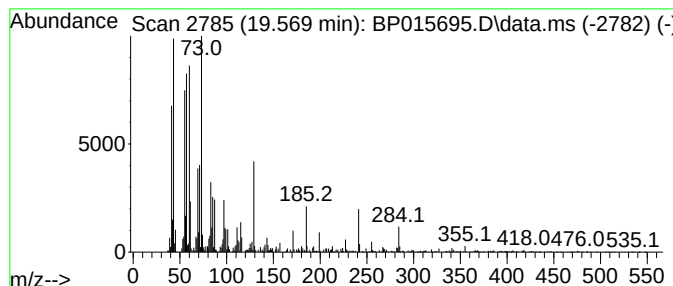
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.569	2.68 ng/ul	231506	Chrysene-d12	21.581

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	99
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	93



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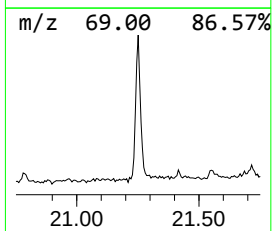
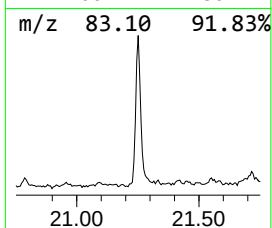
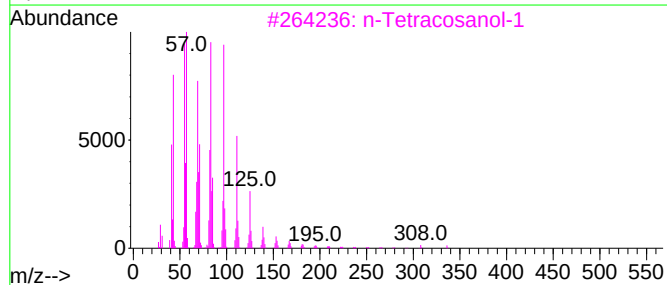
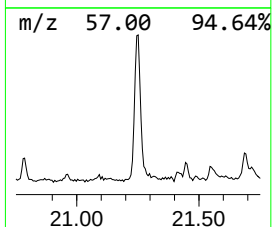
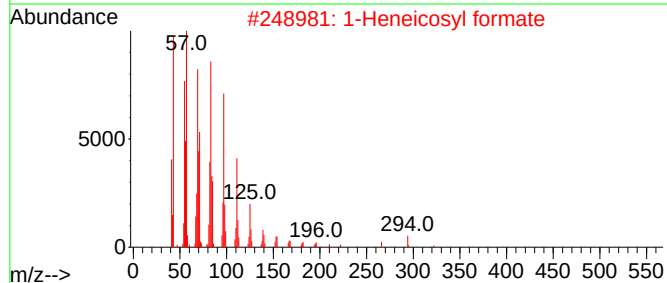
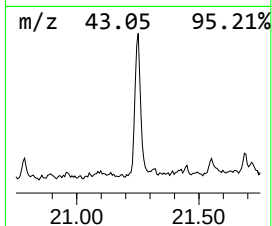
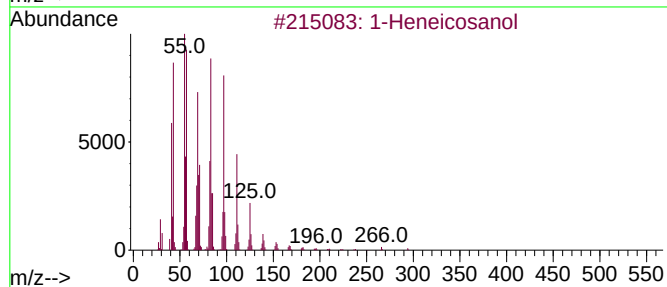
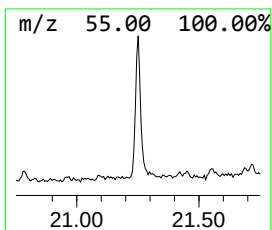
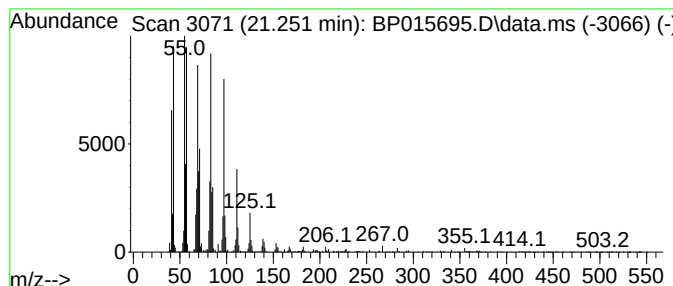
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.251	9.38 ng/ul	809590	Chrysene-d12	21.581

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
Operator : MA/JU
Sample : 03085-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

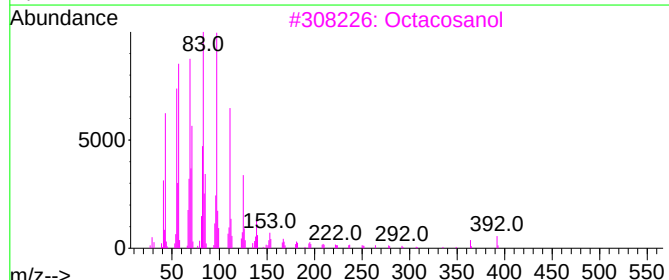
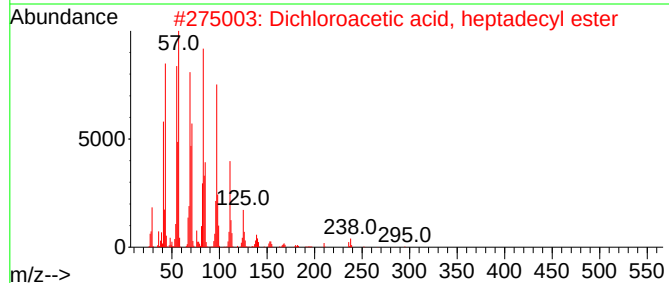
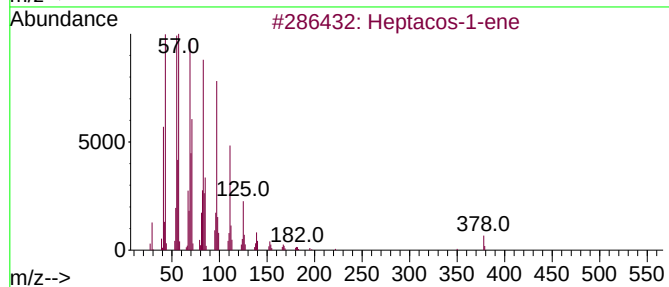
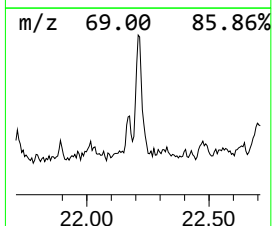
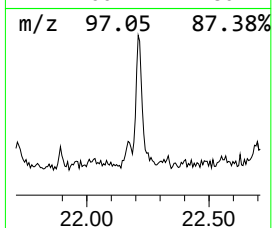
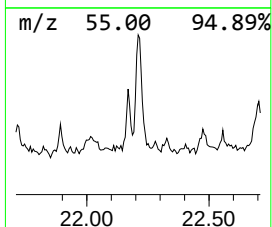
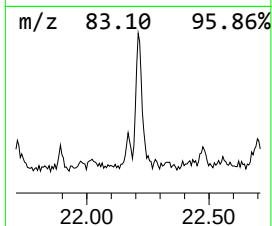
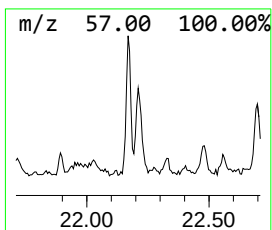
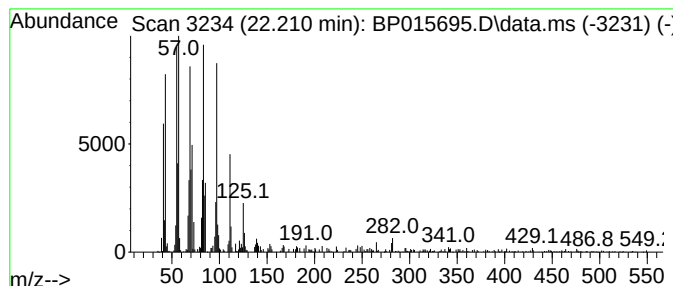
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.210	3.86 ng/ul	333420	Chrysene-d12	21.581	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacos-1-ene	378	C27H54	015306-27-1	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	Octacosanol	410	C28H58O	000557-61-9	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
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Sample : 03085-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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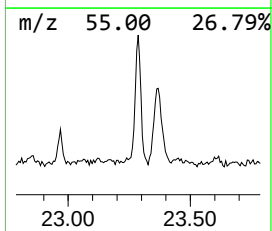
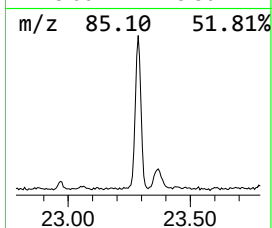
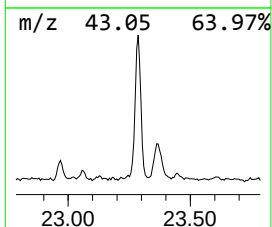
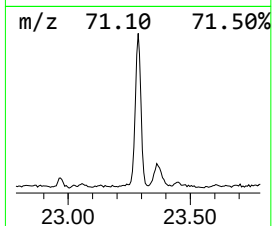
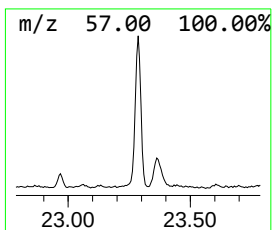
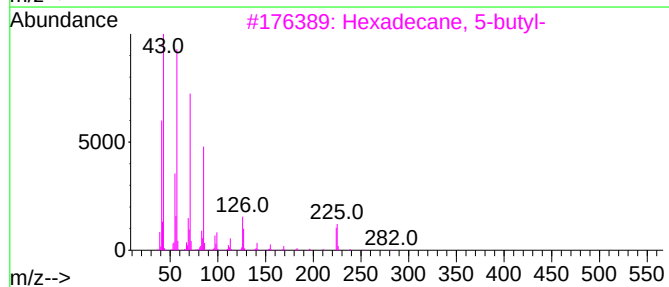
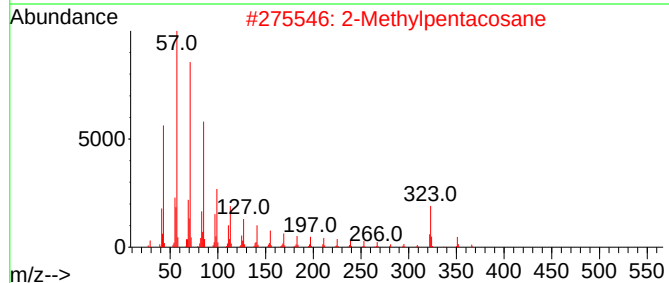
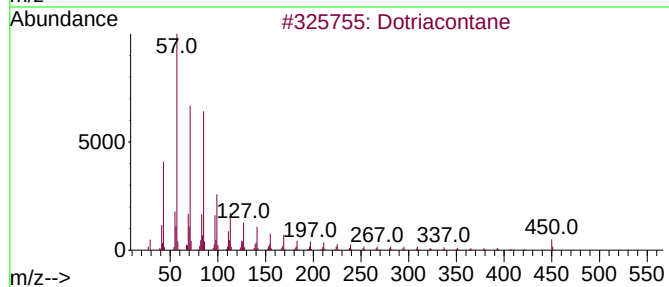
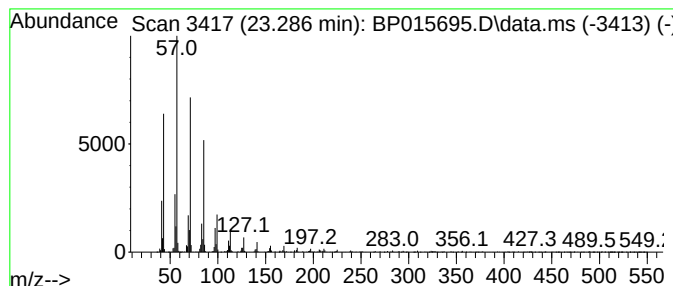
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.286	9.08 ng/ul	847575	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane	451	C32H66	000544-85-4	93
2			2-Methylpentacosane	366	C26H54	000629-87-8	90
3			Hexadecane, 5-butyl-	282	C20H42	006912-07-8	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
Operator : MA/JU
Sample : 03085-04
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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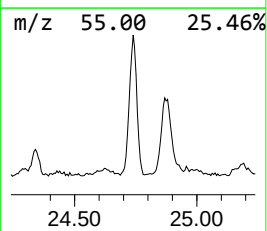
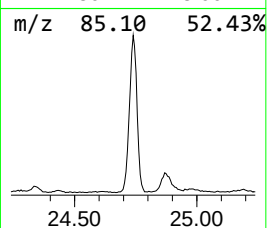
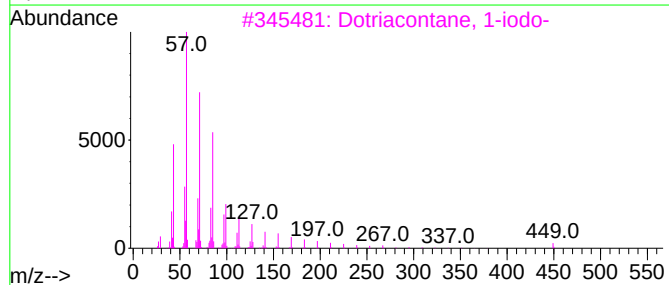
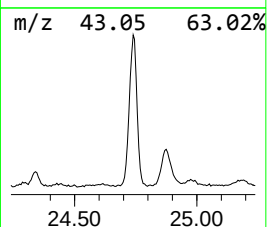
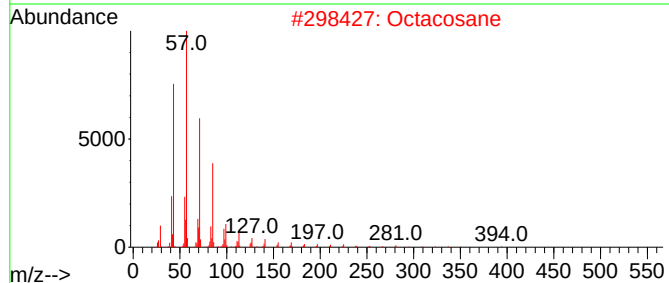
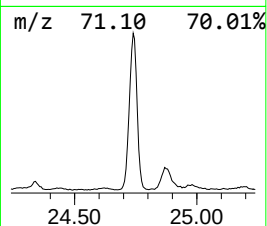
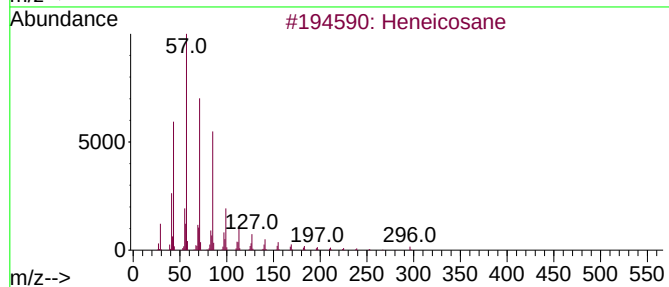
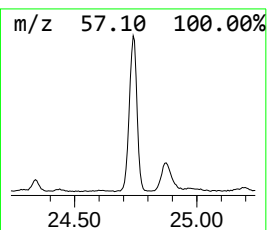
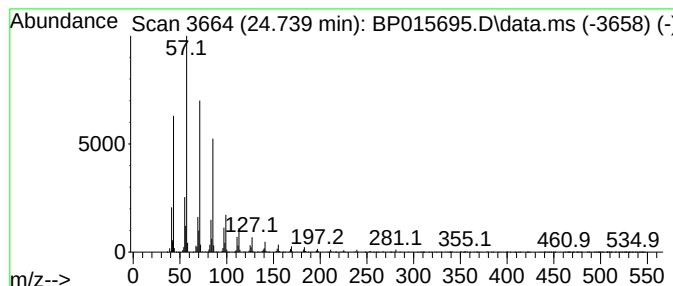
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.739	23.27 ng/ul	2171740	Perylene-d12	24.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
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Misc :
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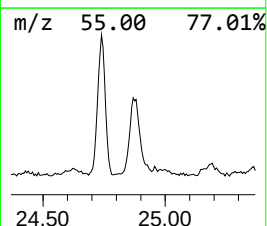
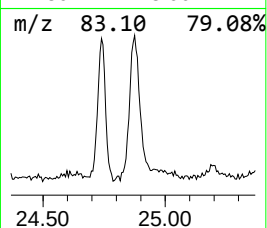
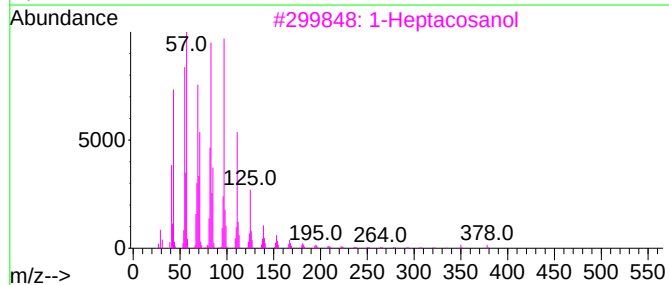
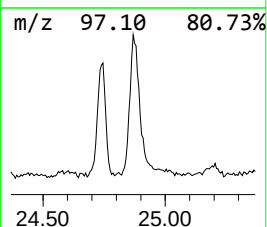
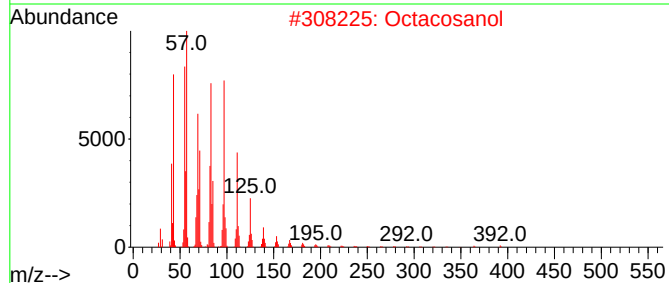
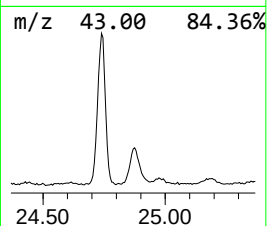
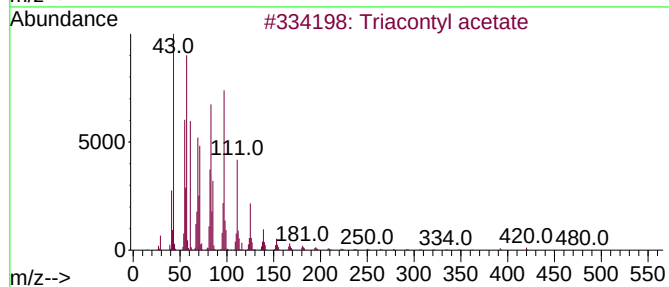
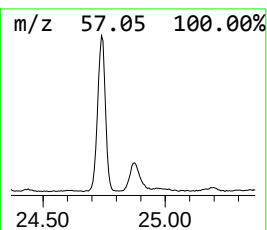
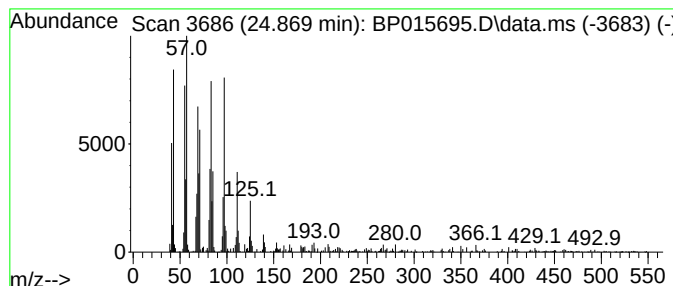
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 Triacontyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.869	8.95 ng/ul	835097	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontyl acetate	480	C32H64O2	041755-58-2	97
2			Octacosanol	410	C28H58O	000557-61-9	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	93
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
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Sample : 03085-04
Misc :
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ClientSampleId :
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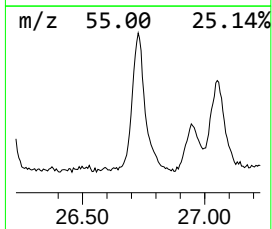
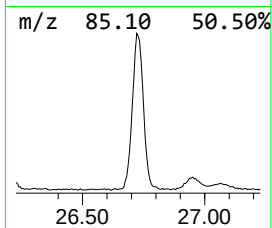
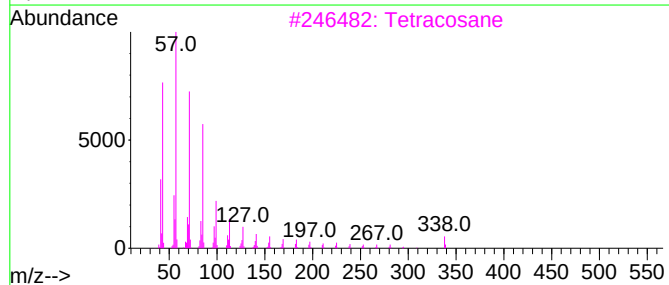
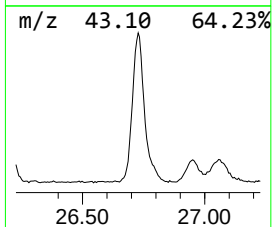
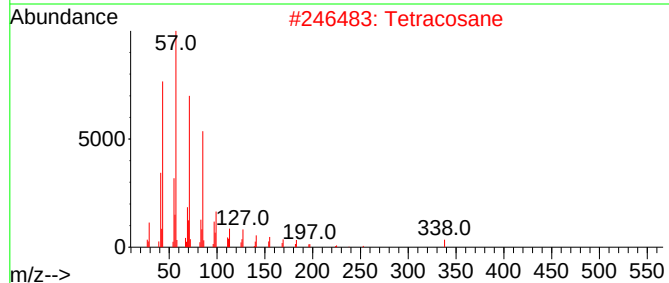
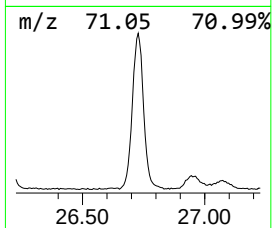
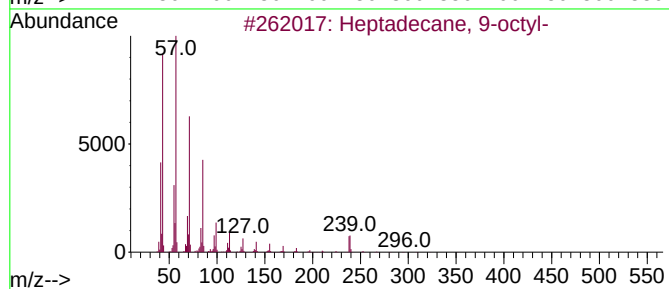
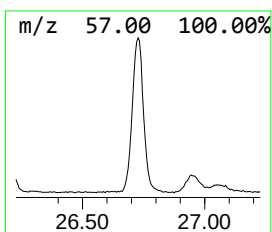
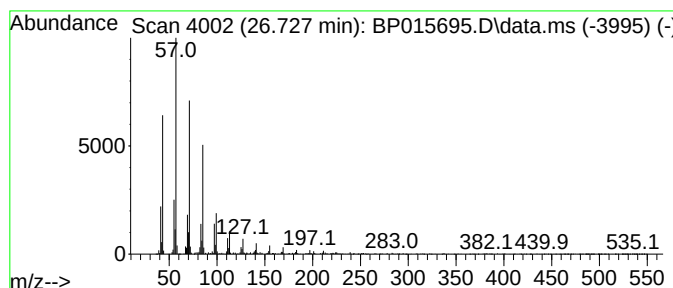
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Quant Title : SVOA CALIBRATION

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.727	35.39 ng/ul	3302280	Perylene-d12	24.139

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2		Tetracosane	338	C24H50	000646-31-1	95
3		Tetracosane	338	C24H50	000646-31-1	94
4		Heptacosane	380	C27H56	000593-49-7	93
5		2-Methylpentacosane	366	C26H54	000629-87-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
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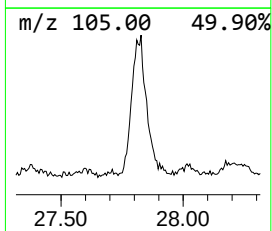
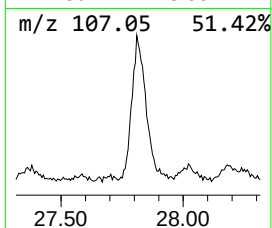
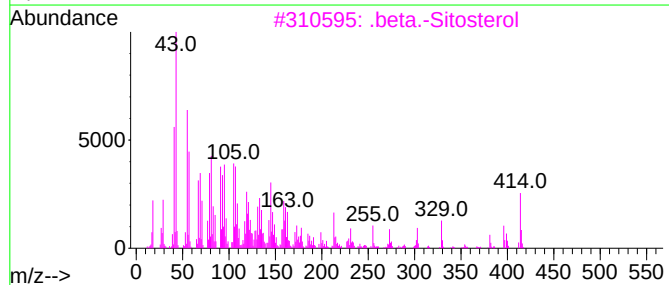
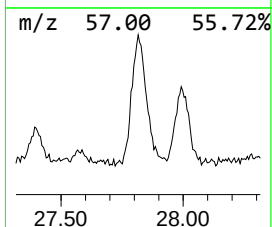
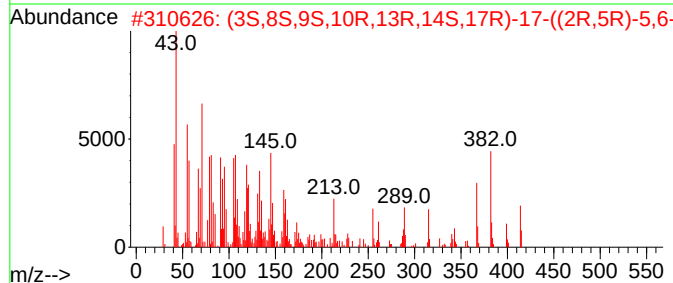
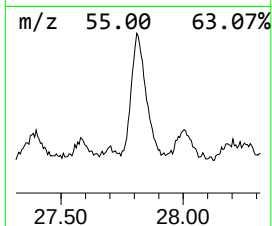
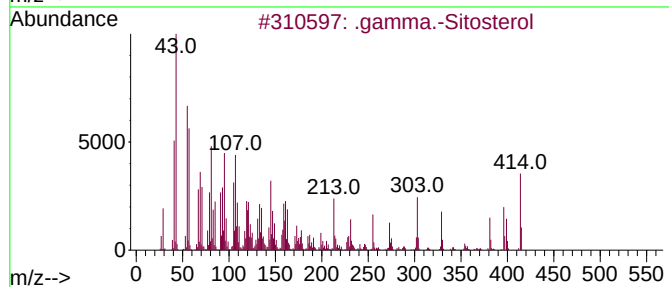
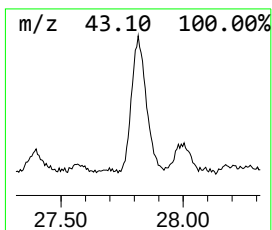
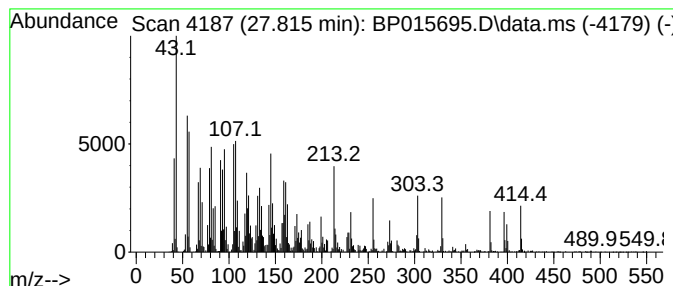
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Quant Title : SVOA CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.815	36.52 ng/ul	3407580	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2			(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414	C29H50O	029365-29-5	64
3			.beta.-Sitosterol	414	C29H50O	000083-46-5	58
4			.beta.-Sitosterol	414	C29H50O	000083-46-5	55
5			Campesterol	400	C28H48O	000474-62-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
Data File : BP015695.D
Acq On : 24 Jun 2023 05:02
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ClientSampleId :
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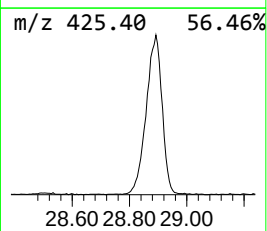
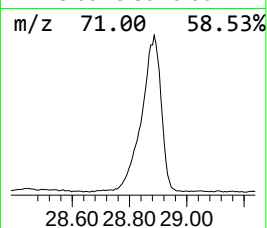
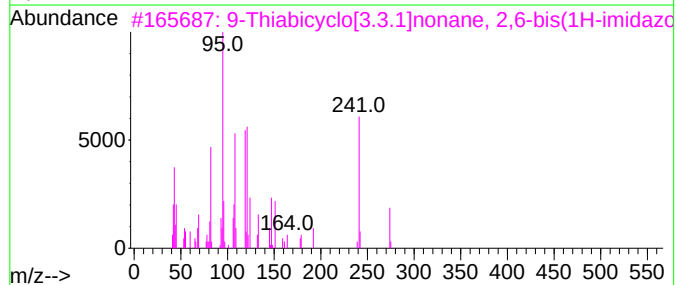
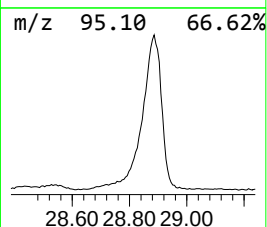
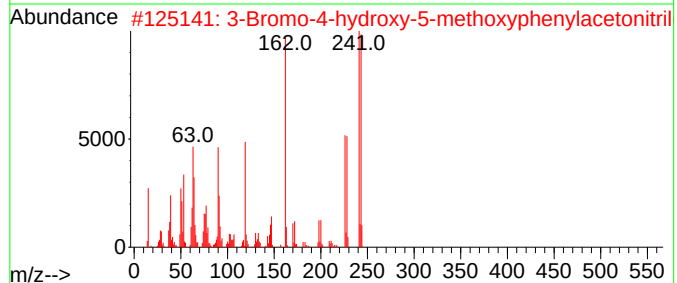
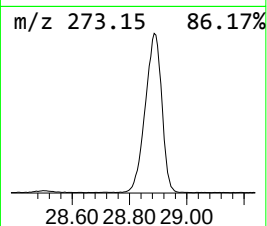
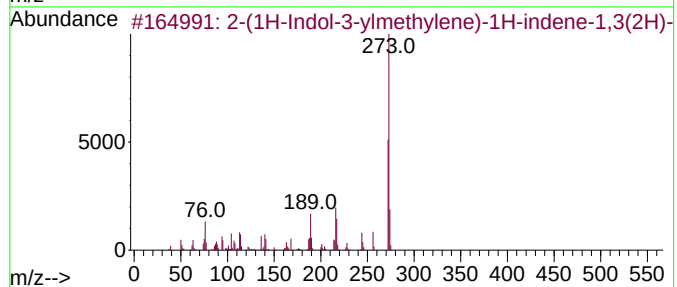
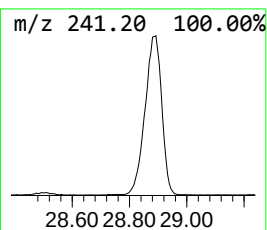
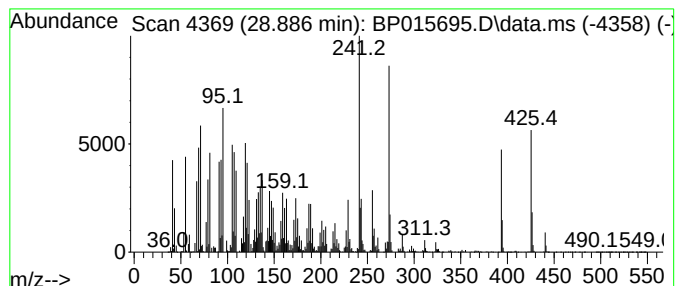
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 12 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.886	183.39 ng/ul	17113300	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	25		
2	3-Bromo-4-hydroxy-5-methoxypheny...	241	C9H8BrNO2	081038-44-0	18		
3	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	18		
4	6-Nitro-2-phenylthieno[2,3-d]pyr...	273	C12H7N3O3S	1000460-07-6	15		
5	8-Nitropyrimido[4,5-b][1,4]benzo...	273	C11H7N5O2S	089046-89-9	15		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062323\
 Data File : BP015695.D
 Acq On : 24 Jun 2023 05:02
 Operator : MA/JU
 Sample : 03085-04
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFP0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP060723.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
Benzophenone	16.093	10.4	ng/ul	636188	3	14.728	1217690	20.0
Methanone, (1-h...	16.651	2.3	ng/ul	159997	4	17.487	1397760	20.0
n-Hexadecanoic ...	18.345	10.2	ng/ul	714193	4	17.487	1397760	20.0
Octadecanoic acid	19.569	2.7	ng/ul	231506	5	21.581	1725570	20.0
1-Heneicosanol	21.251	9.4	ng/ul	809590	5	21.581	1725570	20.0
(DEL) Alkane: S...	22.210	3.9	ng/ul	333420	5	21.581	1725570	20.0
(DEL) Alkane: S...	23.286	9.1	ng/ul	847575	6	24.139	1866310	20.0
(DEL) Alkane: S...	24.739	23.3	ng/ul	2171740	6	24.139	1866310	20.0
Triacetyl acetate	24.869	8.9	ng/ul	835097	6	24.139	1866310	20.0
(DEL) Alkane: S...	26.727	35.4	ng/ul	3302280	6	24.139	1866310	20.0
.gamma.-Sitosterol	27.815	36.5	ng/ul	3407580	6	24.139	1866310	20.0
unknown-01	28.886	183.4	ng/ul	17113300	6	24.139	1866310	20.0