

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
 Data File : BP015792.D
 Acq On : 28 Jun 2023 22:54
 Operator : MA/JU
 Sample : 03142-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFS1

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-BP062623.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BP015792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.381	29	33	44	rVB	67524	107360	0.31%	0.122%
2	3.840	108	111	123	rBV	183675	314093	0.91%	0.357%
3	3.928	123	126	135	rVB	65120	102270	0.30%	0.116%
4	4.046	142	146	150	rBV	39117	55937	0.16%	0.064%
5	4.152	160	164	173	rVB	21844	37014	0.11%	0.042%
6	7.234	681	688	707	rBV	487793	1204331	3.50%	1.369%
7	7.381	707	713	737	rVB	616939	1138108	3.31%	1.293%
8	7.587	742	748	770	rBV	753016	1383243	4.02%	1.572%
9	8.058	821	828	842	rBV	930765	1698965	4.94%	1.931%
10	8.793	946	953	972	rBV	388212	1019479	2.96%	1.158%
11	9.246	1023	1030	1046	rBV	601353	1264981	3.68%	1.437%
12	9.975	1146	1154	1175	rBV	418543	1035129	3.01%	1.176%
13	10.552	1244	1252	1277	rBV	383675	1348300	3.92%	1.532%
14	10.887	1301	1309	1328	rBV	1160451	2265788	6.59%	2.575%
15	11.081	1334	1342	1367	rBV3	103840	428812	1.25%	0.487%
16	13.587	1760	1768	1778	rVV4	19734	41573	0.12%	0.047%
17	14.116	1852	1858	1871	rBV	1095972	1863334	5.42%	2.117%
18	14.404	1897	1907	1921	rBV	1397456	2326577	6.76%	2.644%
19	14.704	1951	1958	1974	rBV	1483034	2421009	7.04%	2.751%
20	15.704	2121	2128	2142	rBV	1502871	2644082	7.69%	3.005%
21	15.875	2151	2157	2177	rVB	193495	530696	1.54%	0.603%
22	16.075	2185	2191	2207	rBV	478418	852060	2.48%	0.968%
23	16.404	2241	2247	2252	rBV5	20797	53543	0.16%	0.061%
24	16.634	2282	2286	2294	rVB	36374	65039	0.19%	0.074%
25	17.340	2402	2406	2413	rBV2	47444	80195	0.23%	0.091%
26	17.410	2414	2418	2422	rBV5	29978	44574	0.13%	0.051%
27	17.469	2422	2428	2433	rBV	1516372	2312152	6.72%	2.627%
28	17.569	2440	2445	2466	rVB2	1272129	2335530	6.79%	2.654%
29	18.263	2557	2563	2568	rBV2	347352	594545	1.73%	0.676%
30	18.322	2568	2573	2582	rVV	1661173	2164785	6.29%	2.460%
31	19.410	2754	2758	2759	rBV	91702	103213	0.30%	0.117%
32	19.469	2763	2768	2777	rVV	385740	720830	2.10%	0.819%
33	19.545	2777	2781	2799	rVV	543113	920107	2.67%	1.046%
34	19.792	2818	2823	2836	rVB2	2066704	3386848	9.84%	3.849%
35	20.269	2902	2904	2908	rVB2	117041	118724	0.35%	0.135%
36	20.757	2984	2987	2992	rBV3	105709	139012	0.40%	0.158%

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37	21.222	3061	3066	3073	rBV4	572746	1008594	2.93%	1.146%
38	21.416	3097	3099	3104	rVB	184673	190441	0.55%	0.216%
39	21.557	3118	3123	3127	rBV	1697373	2502980	7.28%	2.844%
40	23.239	3405	3409	3416	rVB	1034664	1667761	4.85%	1.895%
41	23.927	3521	3526	3534	rVB2	1405225	2984945	8.68%	3.392%
42	24.098	3549	3555	3571	rVB	1346202	3176969	9.23%	3.610%
43	24.674	3648	3653	3663	rVB	1230103	2712213	7.88%	3.082%
44	26.645	3982	3988	3997	rBV	842623	2232750	6.49%	2.537%
45	28.798	4341	4354	4368	rVB3	7848201	34402979	100.00%	39.093%

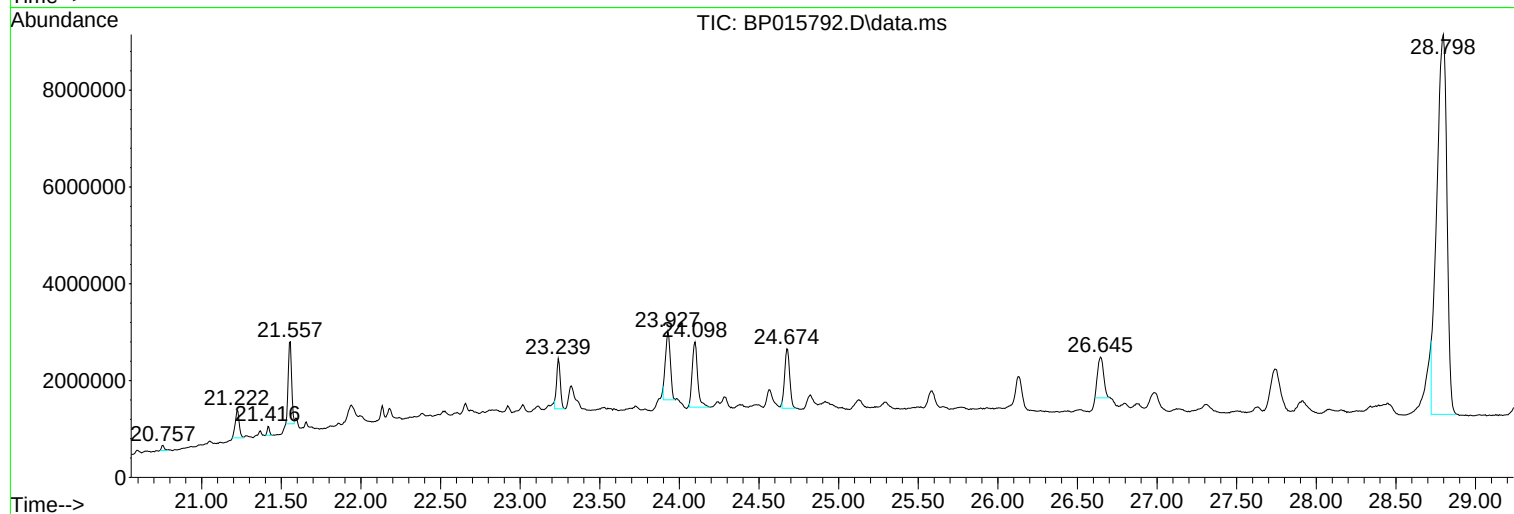
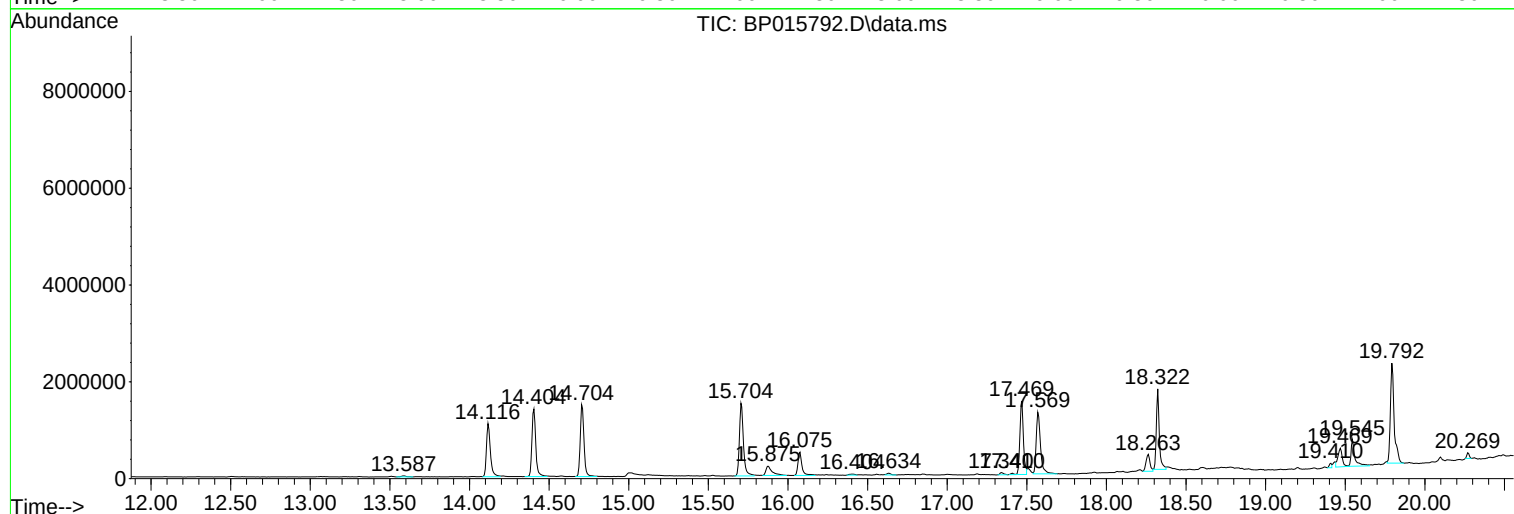
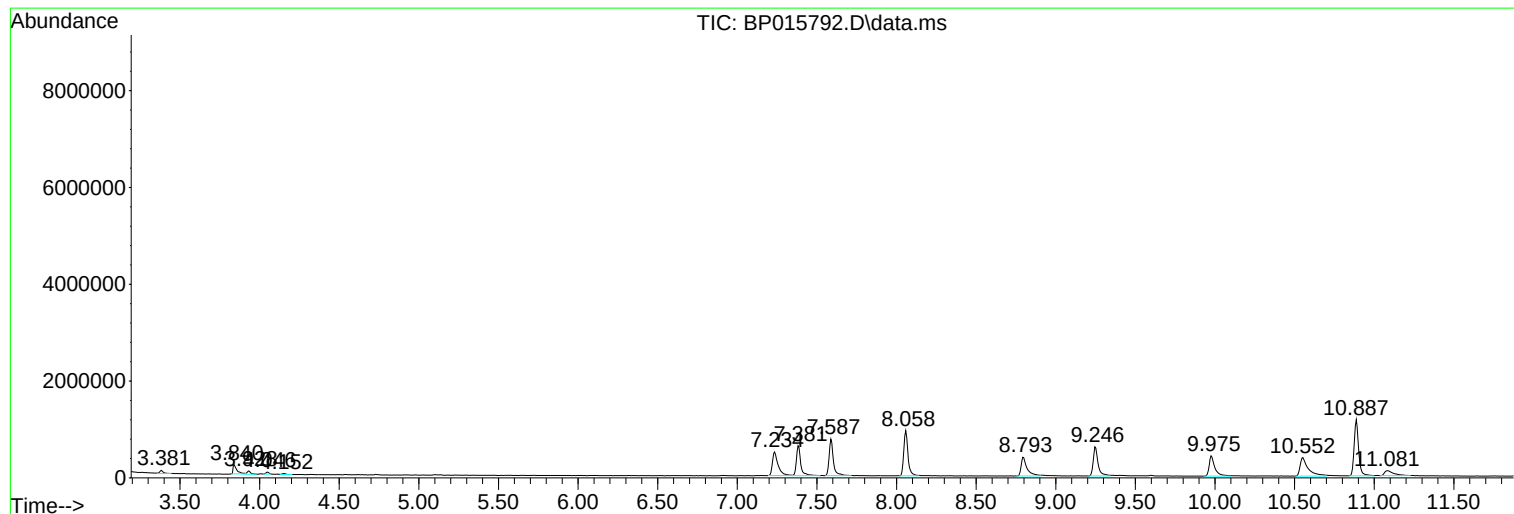
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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



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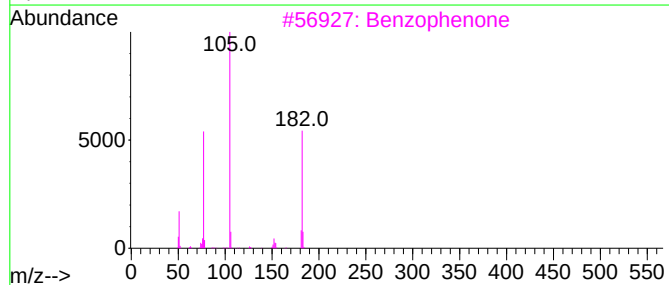
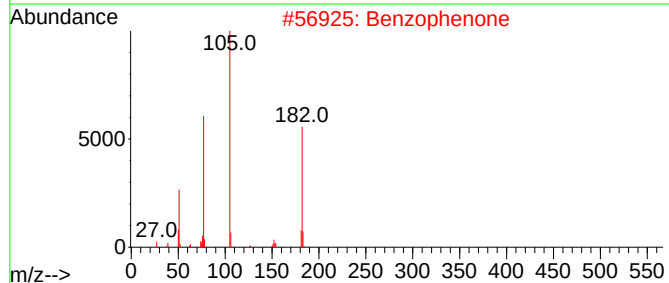
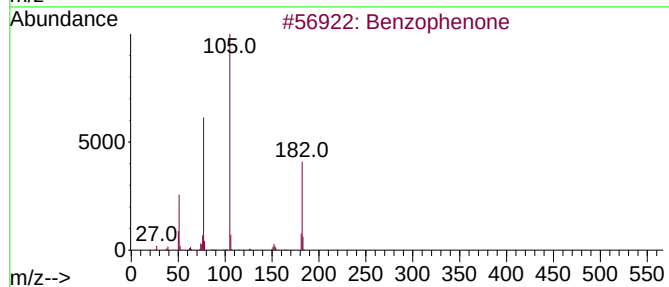
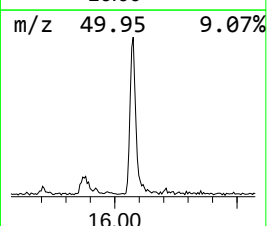
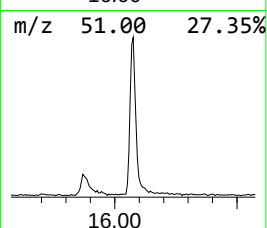
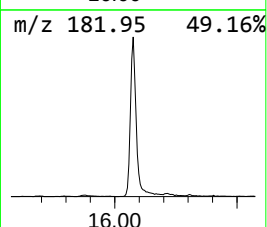
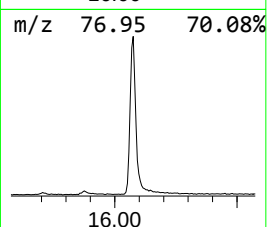
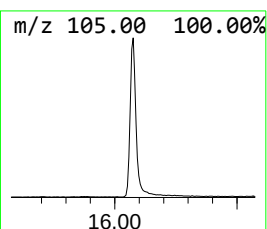
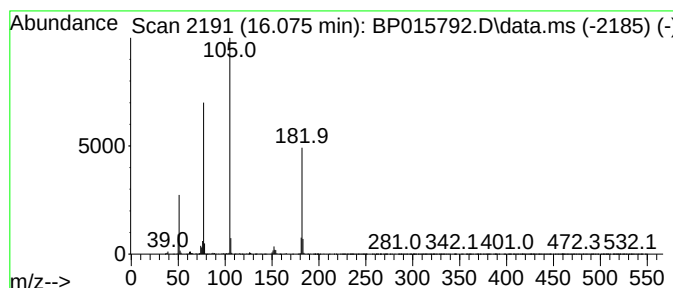
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.075	7.04 ng/ul	852060	Acenaphthene-d10	14.704

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



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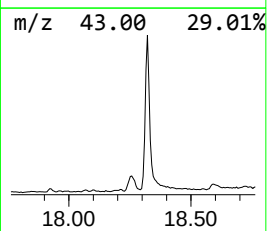
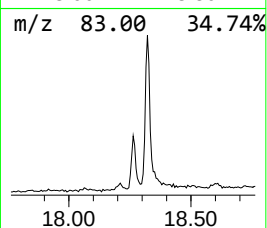
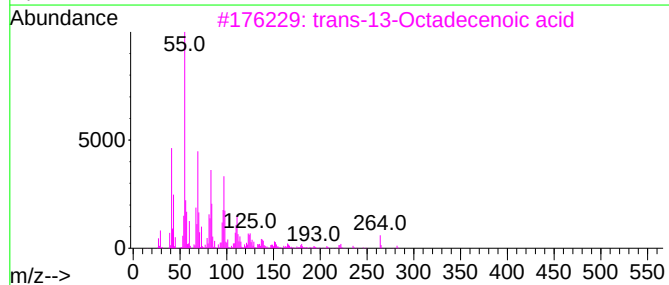
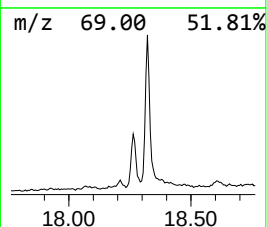
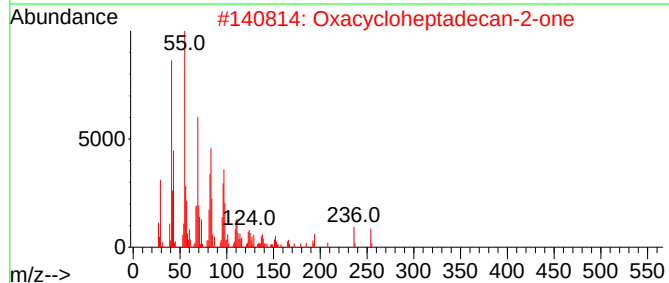
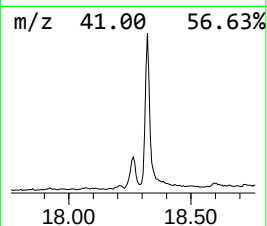
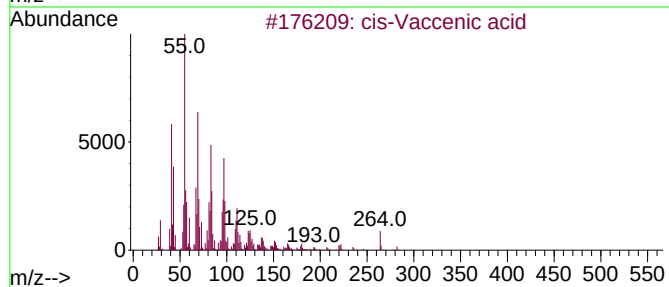
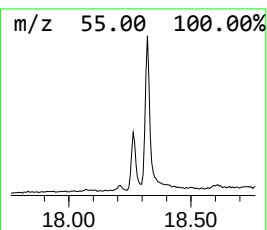
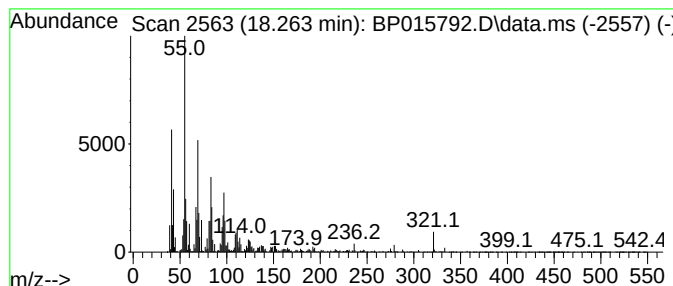
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 cis-Vaccenic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.263	5.14 ng/ul	594545	Phenanthrene-d10	17.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			cis-Vaccenic acid	282	C18H34O2	000506-17-2	87
2			Oxacycloheptadecan-2-one	254	C16H30O2	000109-29-5	86
3			trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	83
4			9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	81
5			cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	80



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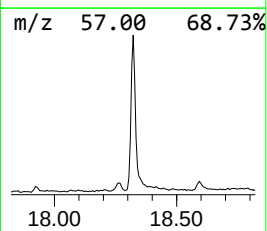
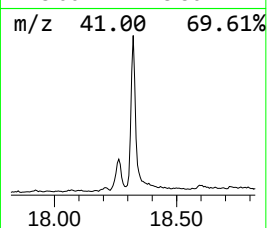
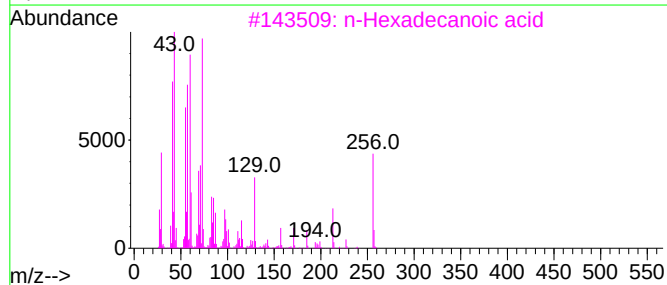
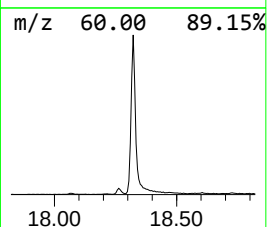
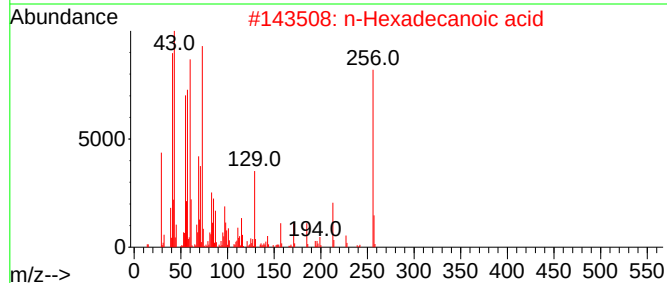
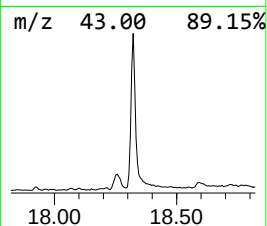
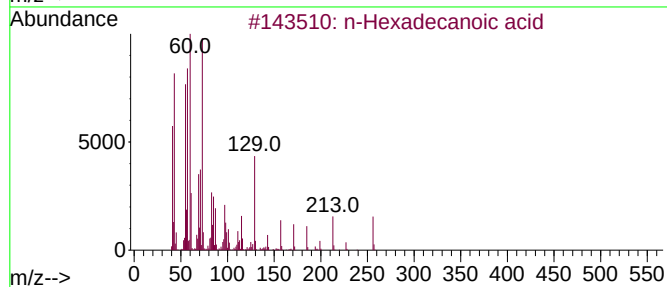
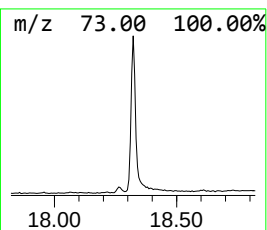
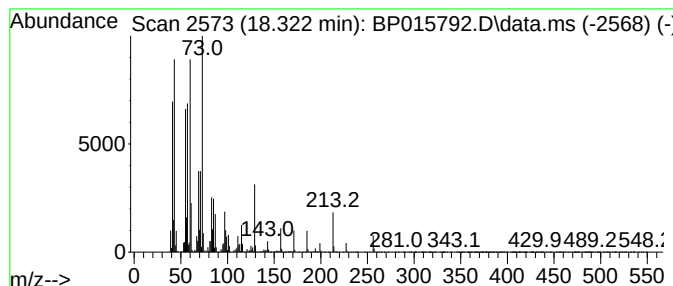
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.322	18.73 ng/ul	2164790	Phenanthrene-d10	17.469

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	98
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91



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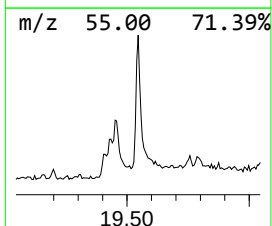
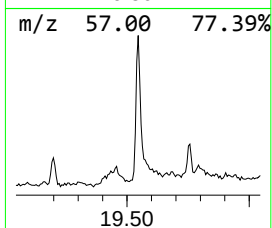
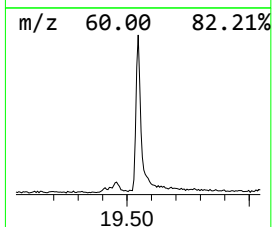
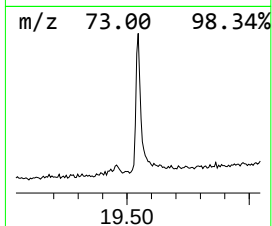
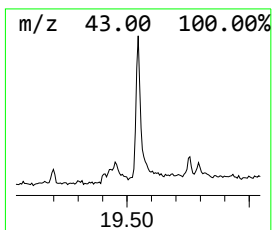
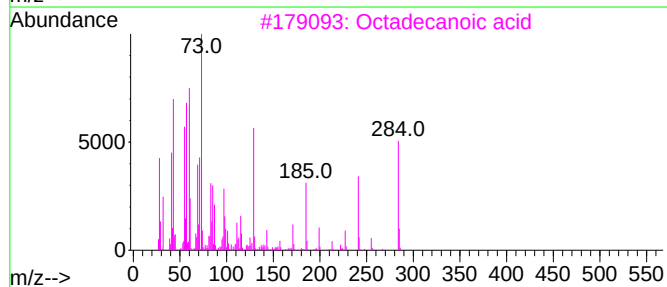
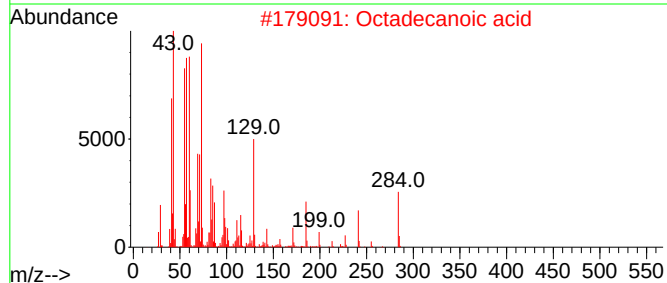
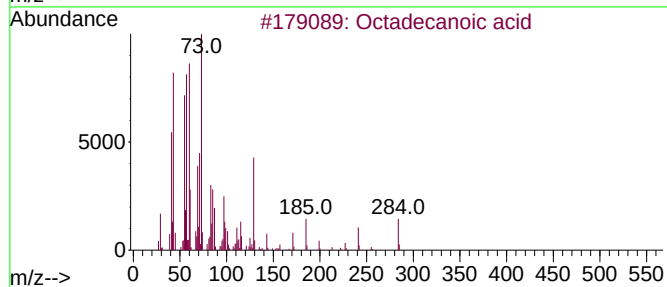
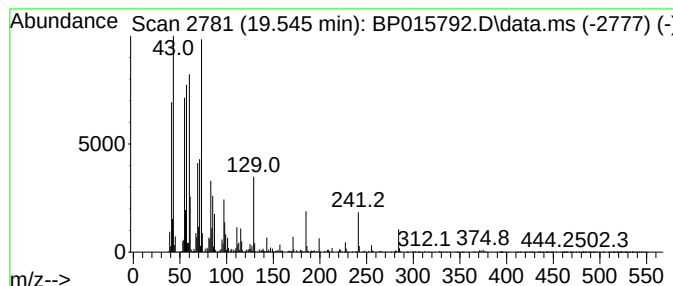
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.545	7.35 ng/ul	920107	Chrysene-d12	21.557

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	97
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	95



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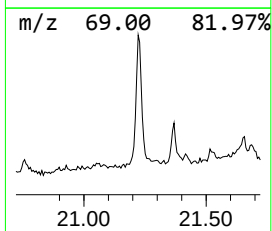
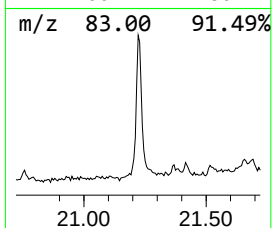
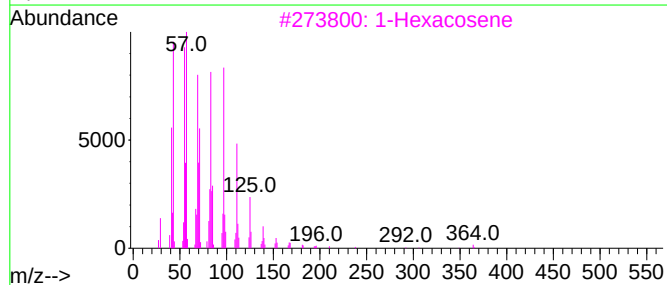
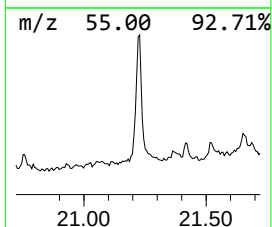
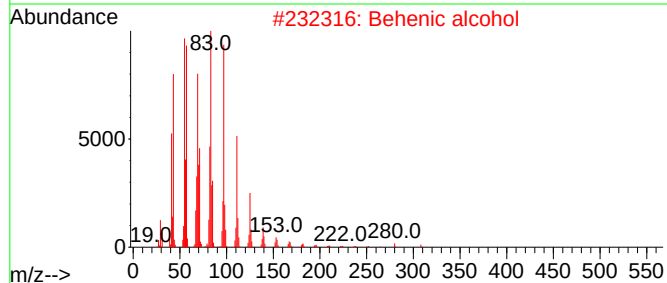
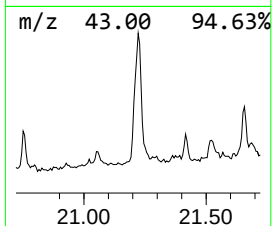
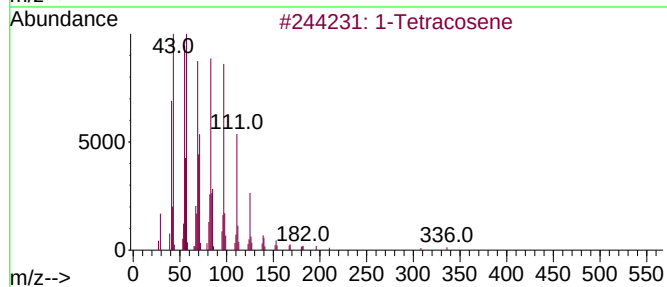
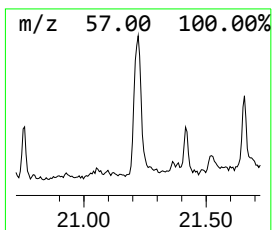
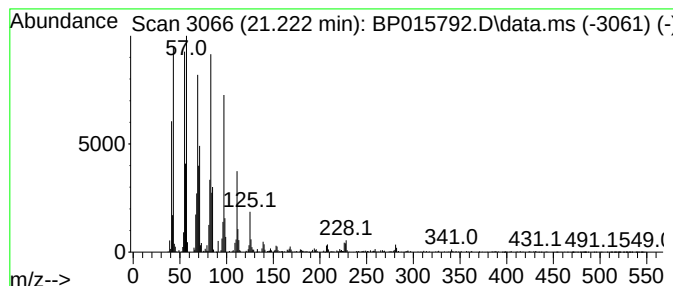
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.222	8.06 ng/ul	1008590	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tetracosene	336	C24H48	010192-32-2	95
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			1-Tricosene	322	C23H46	018835-32-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015792.D
Acq On : 28 Jun 2023 22:54
Operator : MA/JU
Sample : 03142-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS1

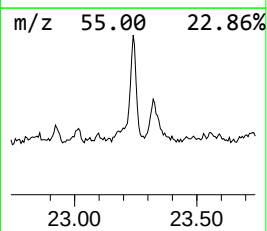
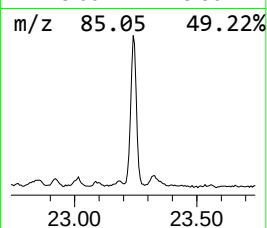
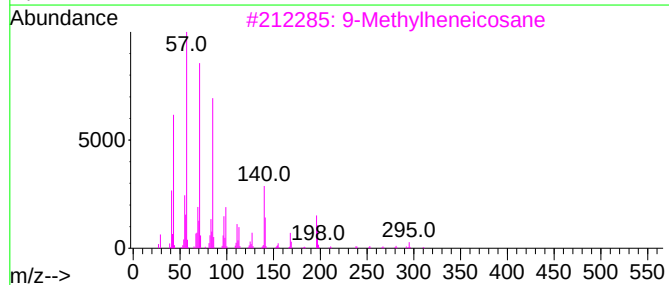
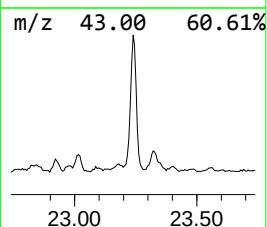
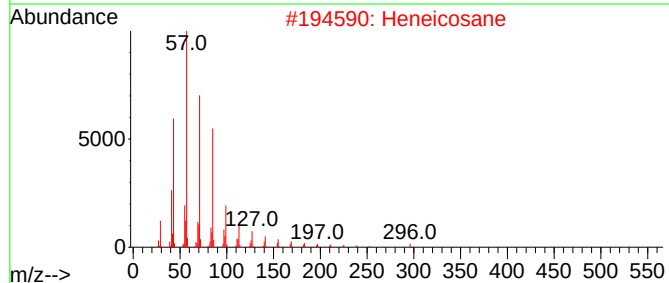
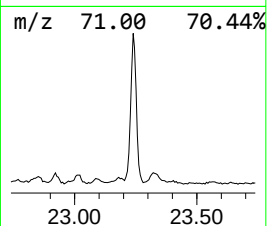
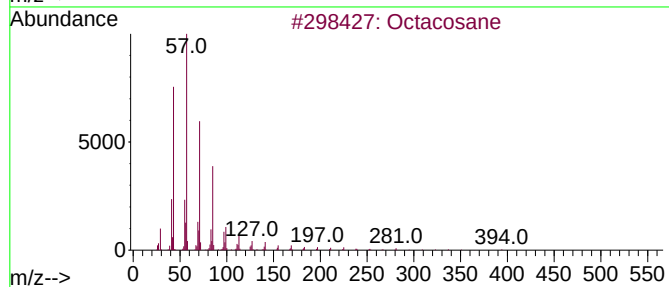
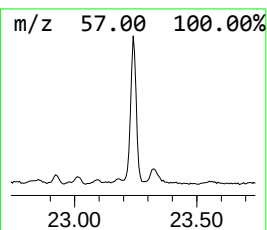
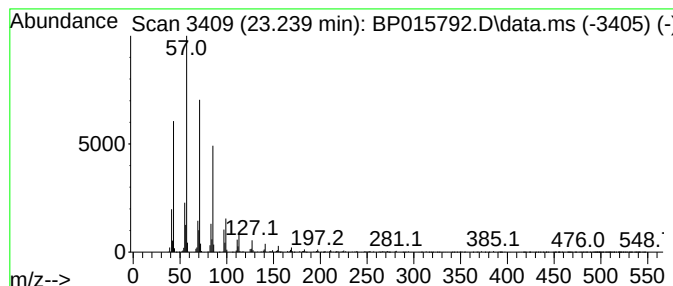
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.239	10.50 ng/ul	1667760	Perylene-d12	24.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			9-Methylheneicosane	310	C22H46	070475-51-3	91
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91
5			Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015792.D
Acq On : 28 Jun 2023 22:54
Operator : MA/JU
Sample : 03142-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS1

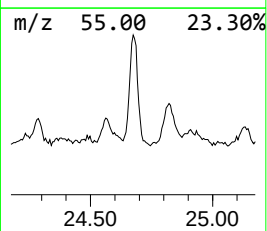
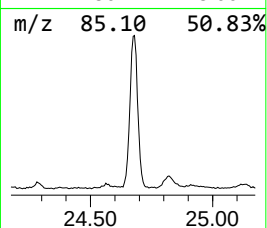
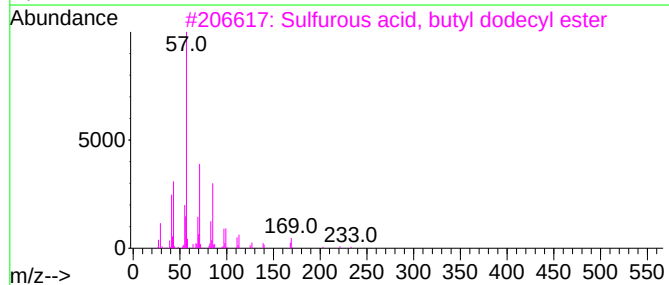
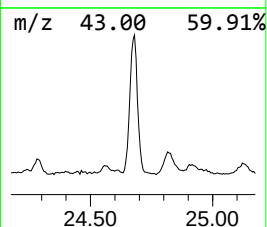
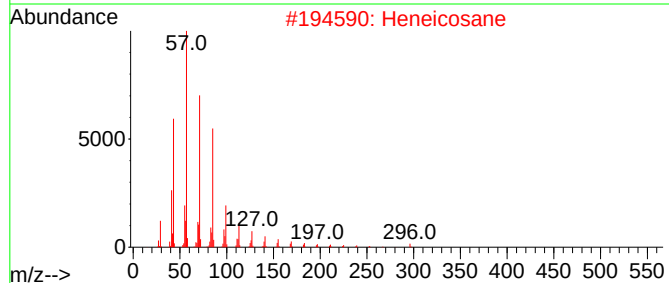
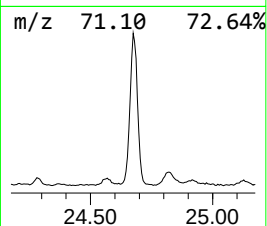
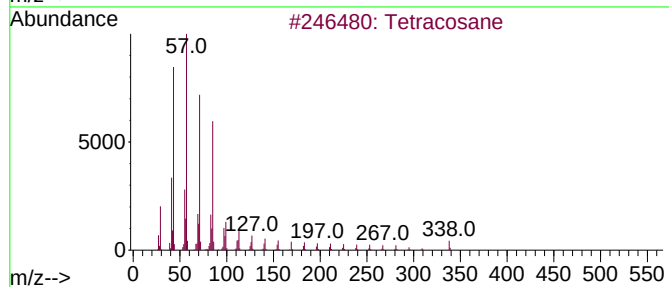
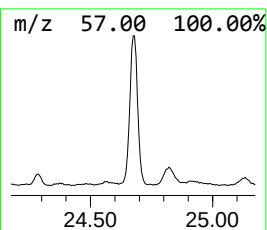
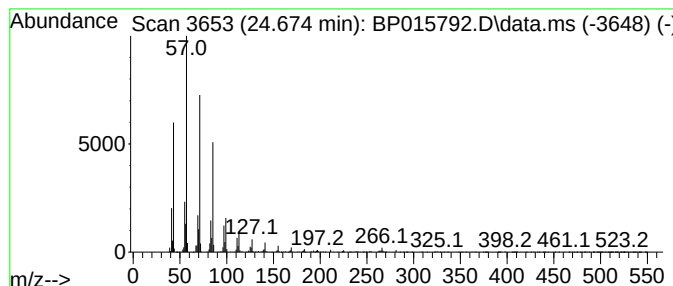
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Quant Title : SVOA CALIBRATION

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.
24.674	17.07 ng/ul	2712210	Perylene-d12	24.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	96
2			Heneicosane	296	C21H44	000629-94-7	91
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
4			Triacontane	422	C30H62	000638-68-6	91
5			Hexatriacontane	507	C36H74	000630-06-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015792.D
Acq On : 28 Jun 2023 22:54
Operator : MA/JU
Sample : 03142-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS1

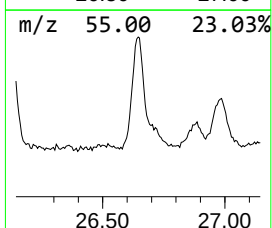
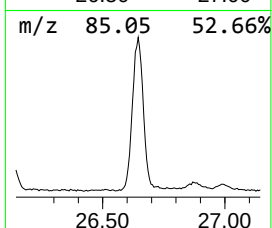
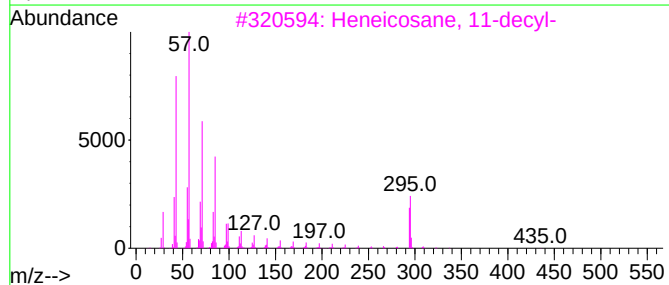
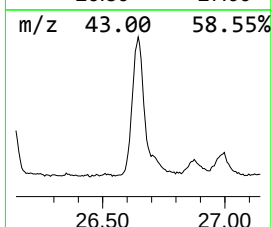
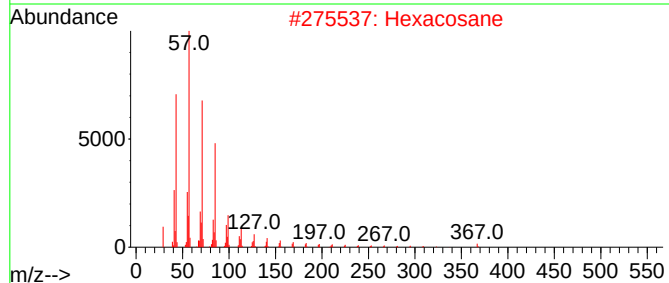
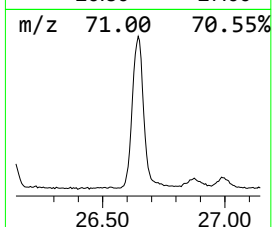
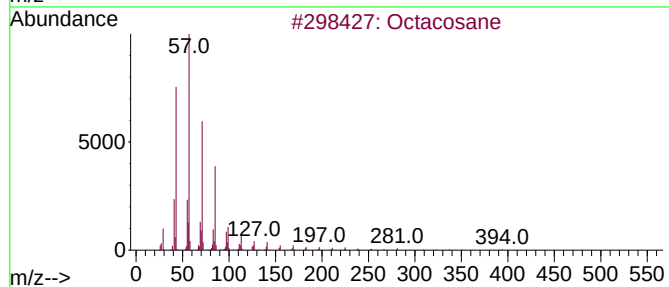
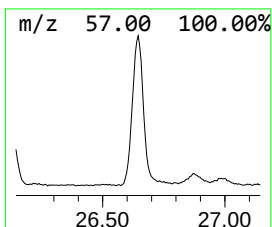
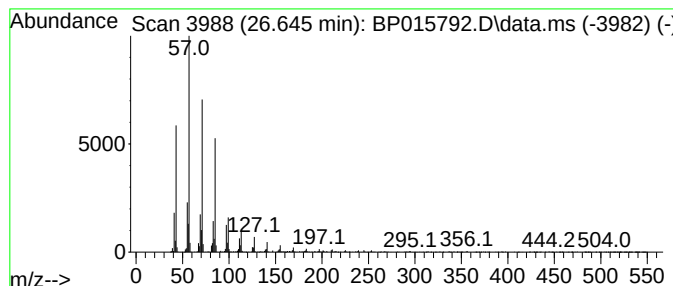
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Quant Title : SVOA CALIBRATION

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.
26.645	14.06 ng/ul	2232750	Perylene-d12	24.098

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015792.D
Acq On : 28 Jun 2023 22:54
Operator : MA/JU
Sample : 03142-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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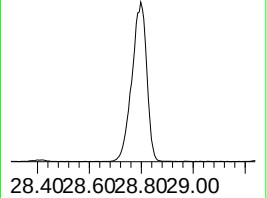
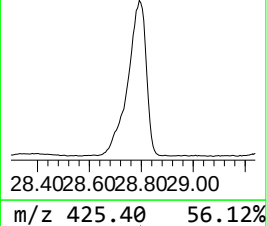
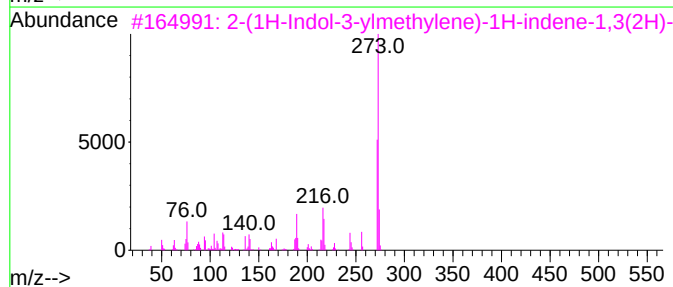
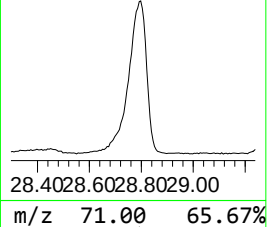
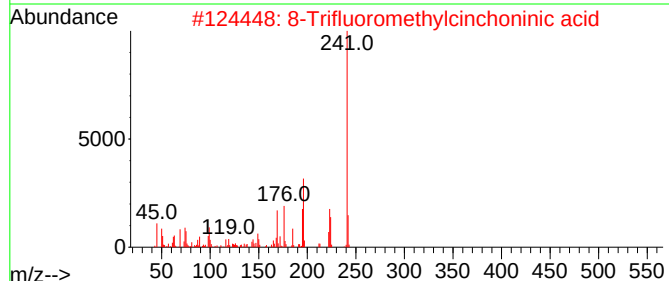
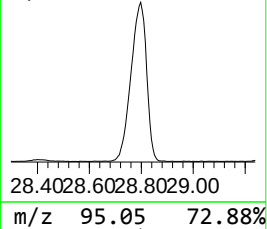
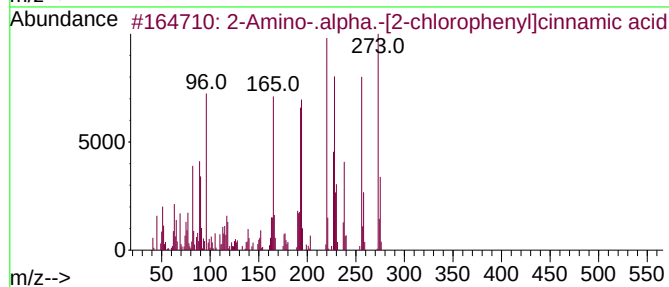
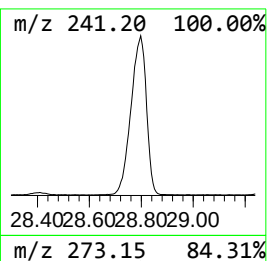
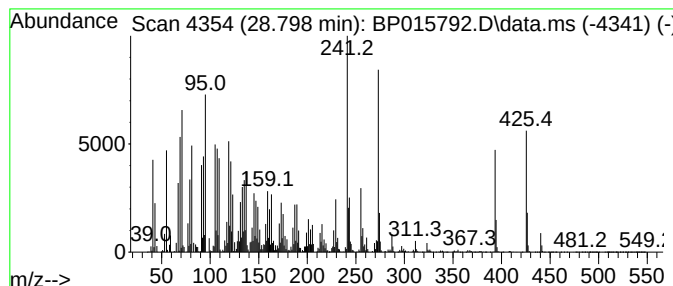
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Quant Title : SVOA CALIBRATION

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

Peak Number 9 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.798	216.58 ng/ul	34403000	Perylene-d12	24.098

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	25		
2	8-Trifluoromethylcinchoninic acid	241	C11H6F3NO2	031009-01-5	25		
3	2-(1H-Indol-3-ylmethylene)-1H-in...	273	C18H11NO2	031060-64-7	15		
4	Adamantane, 1-(4-methylphenylami...	241	C17H23N	019984-39-5	15		
5	Tolcapone	273	C14H11NO5	134308-13-7	15		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062823\
Data File : BP015792.D
Acq On : 28 Jun 2023 22:54
Operator : MA/JU
Sample : 03142-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFS1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	16.075	7.0	ng/ul	852060	3	14.704	2421010	20.0
cis-Vaccenic acid	18.263	5.1	ng/ul	594545	4	17.469	2312150	20.0
n-Hexadecanoic ...	18.322	18.7	ng/ul	2164790	4	17.469	2312150	20.0
Octadecanoic acid	19.545	7.3	ng/ul	920107	5	21.557	2502980	20.0
(DEL) Alkane: S...	21.222	8.1	ng/ul	1008590	5	21.557	2502980	20.0
(DEL) Alkane: S...	23.239	10.5	ng/ul	1667760	6	24.098	3176970	20.0
(DEL) Alkane: S...	24.674	17.1	ng/ul	2712210	6	24.098	3176970	20.0
(DEL) Alkane: S...	26.645	14.1	ng/ul	2232750	6	24.098	3176970	20.0
unknown-01	28.798	216.6	ng/ul	34403000	6	24.098	3176970	20.0