

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
 Data File : BP015809.D
 Acq On : 29 Jun 2023 14:05
 Operator : MA/JU
 Sample : 03143-14
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DCFV1

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: BP015809.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	30	33	38	rVB	26324	32713	0.30%	0.065%
2	3.834	109	110	122	rVV	150758	263675	2.44%	0.520%
3	3.928	122	126	132	rVB	67930	93784	0.87%	0.185%
4	4.046	142	146	153	rVB	28216	48113	0.45%	0.095%
5	4.146	161	163	169	rVB2	17371	23235	0.21%	0.046%
6	4.387	201	204	209	rVB	23086	29879	0.28%	0.059%
7	4.822	274	278	285	rVB9	8459	19264	0.18%	0.038%
8	5.099	322	325	329	rVB4	6800	10827	0.10%	0.021%
9	5.652	416	419	424	rVB6	7010	11043	0.10%	0.022%
10	7.246	681	690	709	rBV	164303	547925	5.07%	1.081%
11	7.387	709	714	729	rVB	221925	446157	4.13%	0.880%
12	7.593	742	749	764	rBV	272931	587967	5.44%	1.160%
13	8.057	822	828	855	rVV	604055	1240018	11.47%	2.447%
14	8.622	920	924	930	rVB9	5651	11978	0.11%	0.024%
15	8.810	949	956	975	rBV	139789	492734	4.56%	0.972%
16	9.263	1026	1033	1047	rBV	207612	543295	5.03%	1.072%
17	9.987	1148	1156	1173	rBV	129800	451708	4.18%	0.891%
18	10.569	1247	1255	1288	rBV2	146681	658984	6.10%	1.300%
19	10.893	1301	1310	1327	rBV	797467	1785909	16.52%	3.524%
20	11.087	1336	1343	1362	rBV2	94456	368359	3.41%	0.727%
21	12.293	1543	1548	1556	rBV2	7465	17708	0.16%	0.035%
22	13.510	1751	1755	1760	rBV7	8176	13399	0.12%	0.026%
23	13.587	1762	1768	1778	rVV	37750	78390	0.73%	0.155%
24	14.122	1850	1859	1872	rBV	536528	1055011	9.76%	2.082%
25	14.404	1900	1907	1924	rBV2	729211	1423309	13.17%	2.809%
26	14.575	1933	1936	1942	rVB7	10503	16178	0.15%	0.032%
27	14.710	1952	1959	1977	rBV	1346318	2198189	20.34%	4.338%
28	15.034	2007	2014	2019	rBV6	40138	110852	1.03%	0.219%
29	15.128	2027	2030	2037	rVB9	19524	33080	0.31%	0.065%
30	15.475	2086	2089	2095	rBV8	8817	17176	0.16%	0.034%
31	15.534	2095	2099	2103	rVV4	14670	17615	0.16%	0.035%
32	15.710	2122	2129	2144	rBV	820134	1592919	14.74%	3.143%
33	15.810	2144	2146	2153	rVV8	17412	32255	0.30%	0.064%
34	15.886	2154	2159	2179	rVV4	80797	265791	2.46%	0.525%
35	16.081	2187	2192	2201	rBV	108488	206527	1.91%	0.408%
36	17.186	2377	2380	2385	rBV4	16027	21008	0.19%	0.041%

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37	17.469	2422	2428	2441	rBV	1467877	2544048	23.54%	5.020%
38	17.575	2441	2446	2466	rVB2	840456	1629655	15.08%	3.216%
39	18.251	2557	2561	2569	rBV2	221953	383669	3.55%	0.757%
40	18.322	2569	2573	2582	rBV	799395	1130439	10.46%	2.231%
41	19.204	2720	2723	2728	rBV2	42769	76348	0.71%	0.151%
42	19.410	2755	2758	2759	rBV3	58085	56569	0.52%	0.112%
43	19.433	2760	2762	2764	rVV2	87072	100854	0.93%	0.199%
44	19.475	2764	2769	2776	rVB	482750	765690	7.08%	1.511%
45	19.545	2777	2781	2787	rBV2	337535	526635	4.87%	1.039%
46	19.798	2813	2824	2827	rBV	1339157	2329370	21.55%	4.597%
47	20.274	2902	2905	2909	rBV3	126359	145980	1.35%	0.288%
48	21.227	3061	3067	3073	rBV4	488352	979358	9.06%	1.933%
49	21.557	3118	3123	3128	rBV	1710229	2633002	24.36%	5.196%
50	22.133	3219	3221	3225	rBV	317804	345634	3.20%	0.682%
51	22.439	3270	3273	3277	rVB	376051	470140	4.35%	0.928%
52	23.245	3405	3410	3416	rVB	1401879	2292489	21.21%	4.524%
53	23.327	3419	3424	3441	rVB3	643081	1915575	17.72%	3.780%
54	24.104	3550	3556	3575	rVB	1155963	2976341	27.54%	5.874%
55	24.680	3648	3654	3662	rVB	1735095	3795532	35.11%	7.490%
56	28.774	4343	4350	4370	rVB3	2904718	10809175	100.00%	21.331%

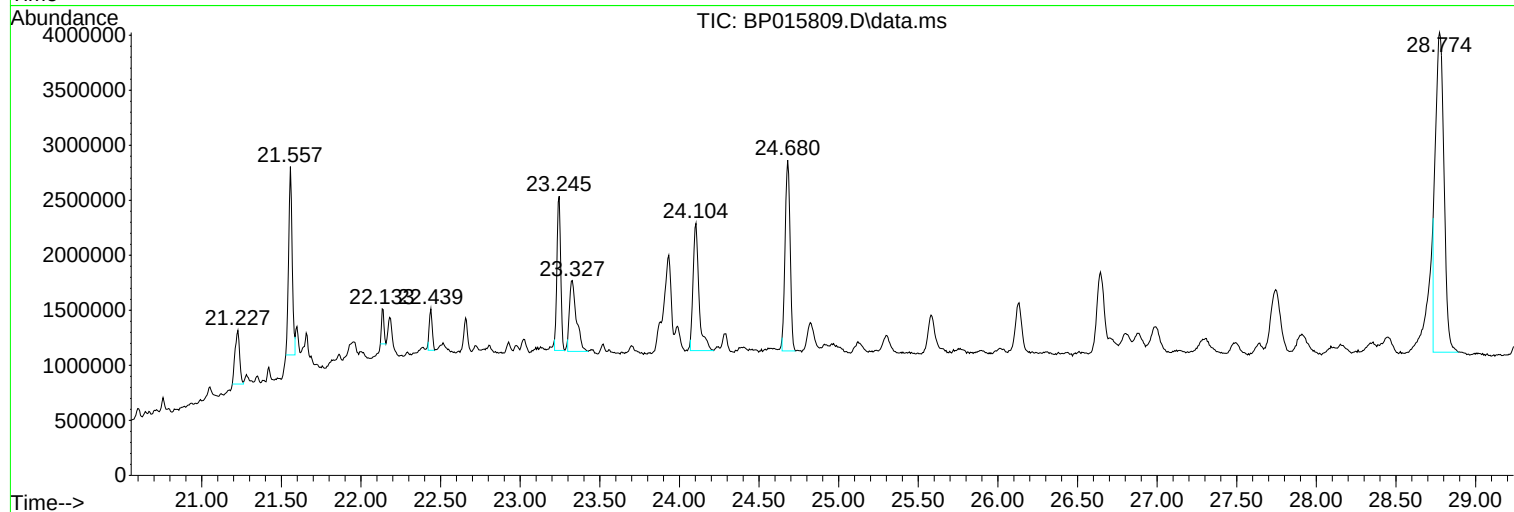
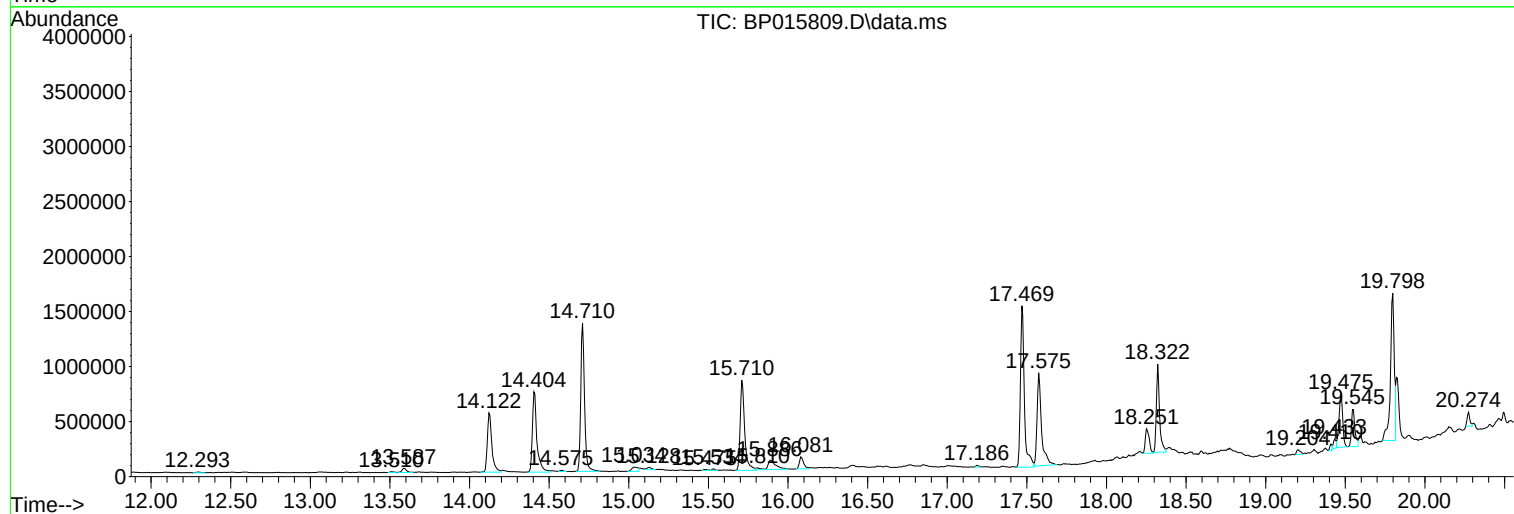
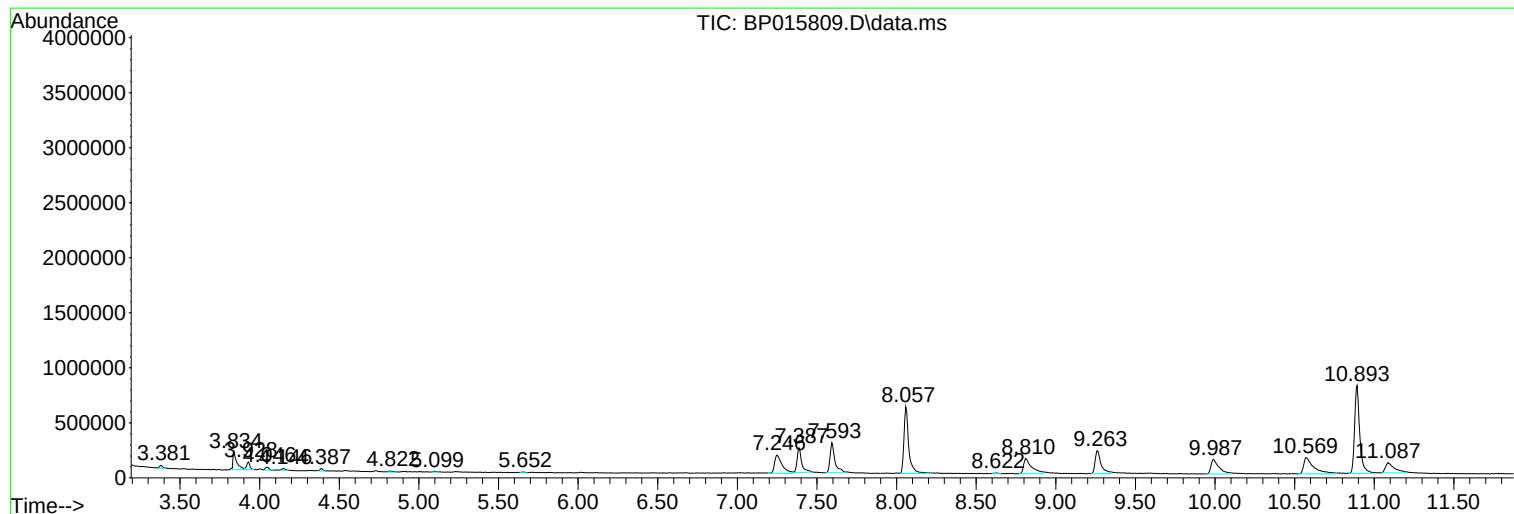
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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



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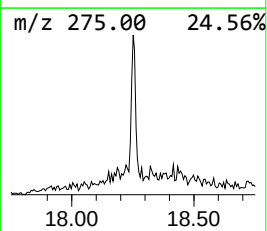
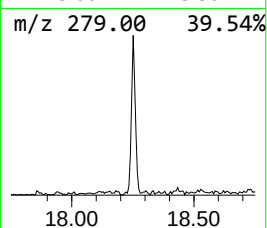
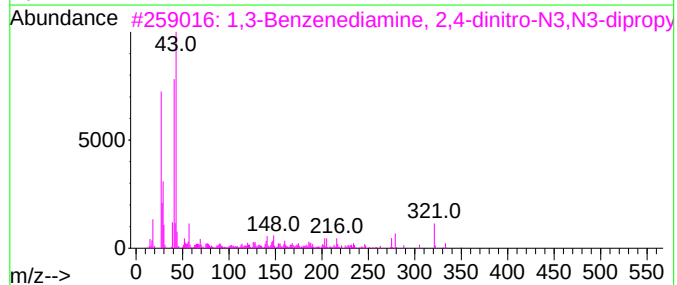
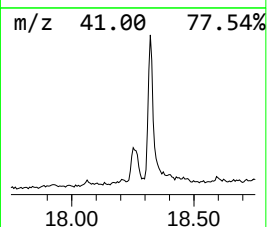
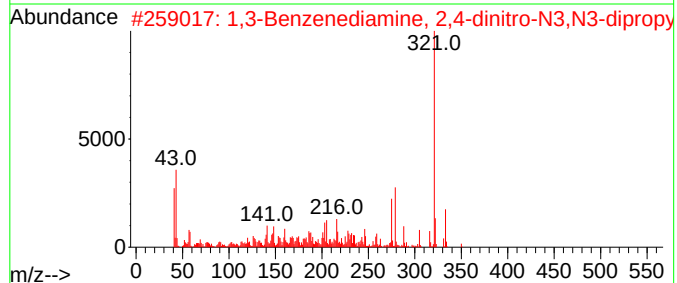
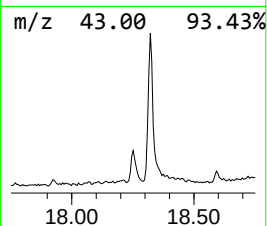
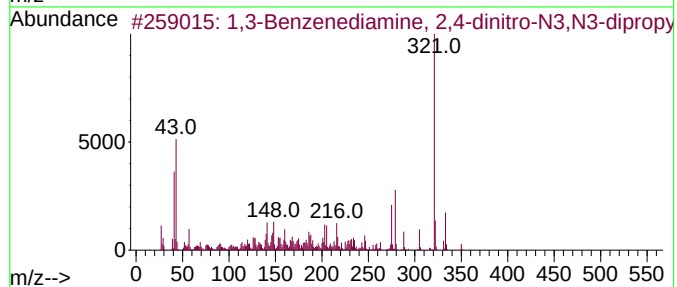
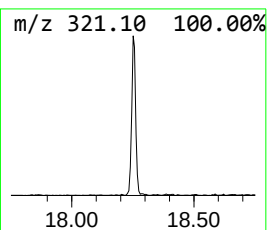
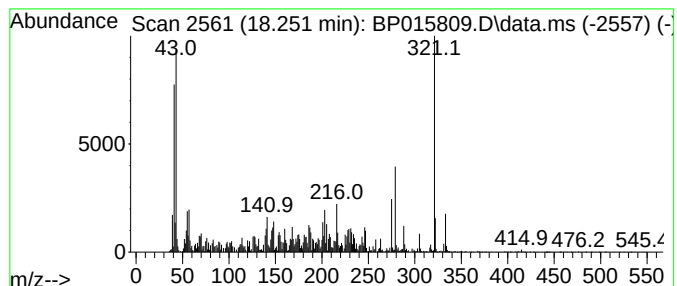
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 1,3-Benzenediamine, 2,4-din... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.251	3.02 ng/ul	383669	Phenanthrene-d10	17.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenediamine, 2,4-dinitro-...	350	C13H17F3N4O4	029091-21-2	87		
2	1,3-Benzenediamine, 2,4-dinitro-...	350	C13H17F3N4O4	029091-21-2	55		
3	1,3-Benzenediamine, 2,4-dinitro-...	350	C13H17F3N4O4	029091-21-2	50		
4	Fumaric acid, monoamide, N-(2,5-...	321	C17H23N05	1000345-40-2	30		
5	propanedinitrile, 2-[[4-(dipheny...	321	C22H15N3	1010402-33-4	27		



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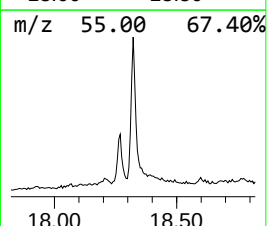
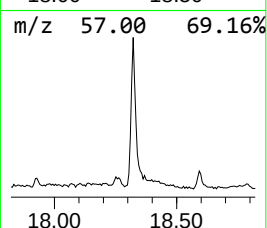
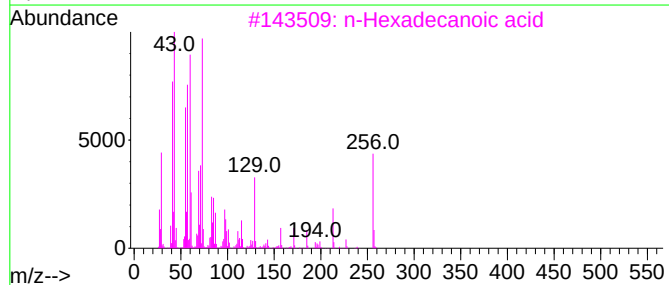
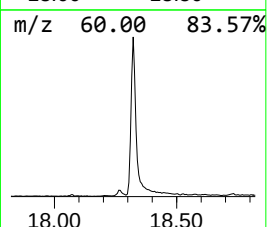
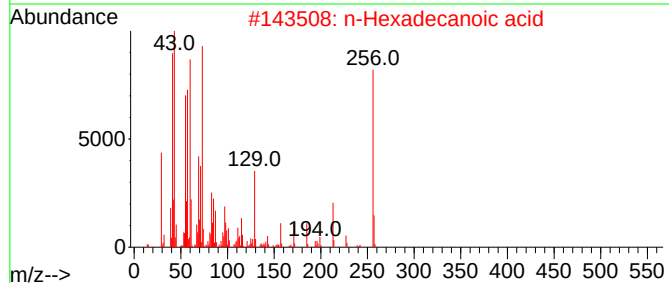
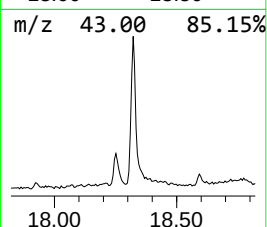
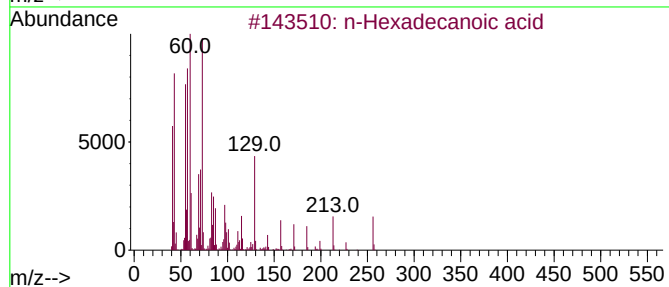
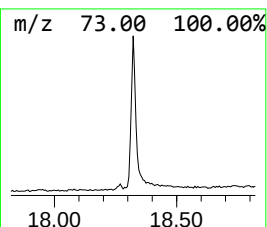
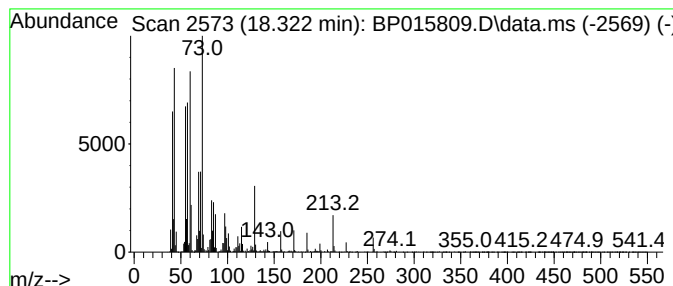
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.322	8.89 ng/ul	1130440	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			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92



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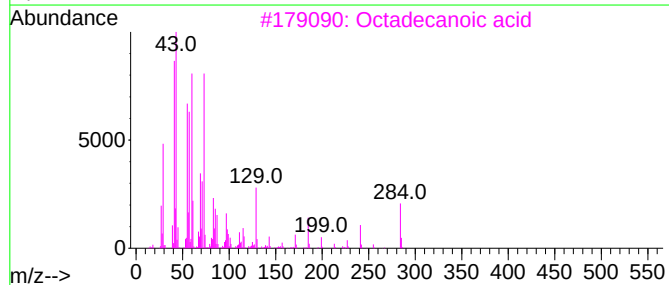
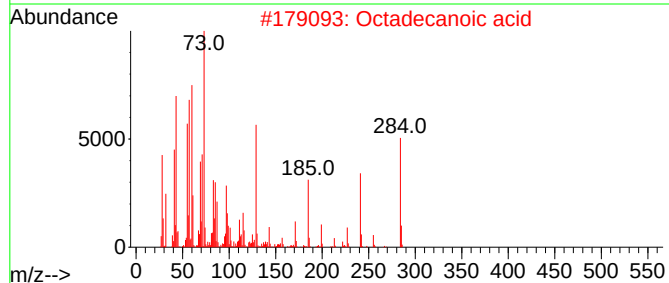
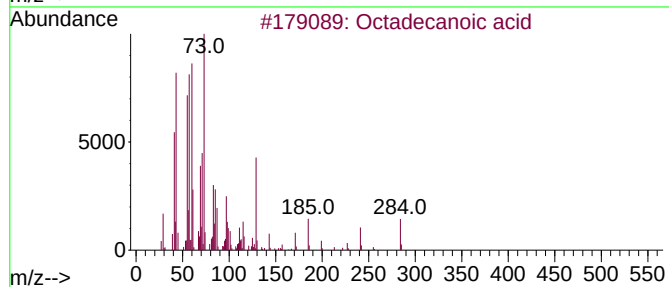
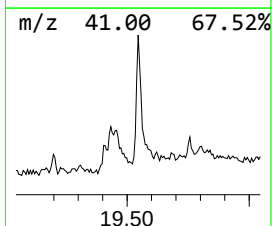
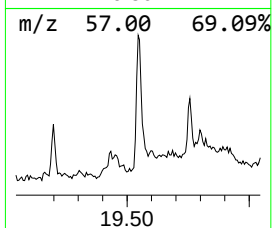
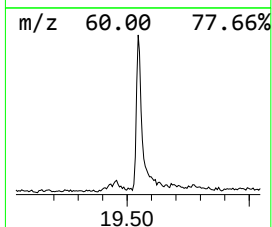
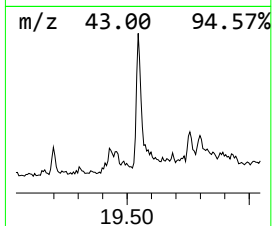
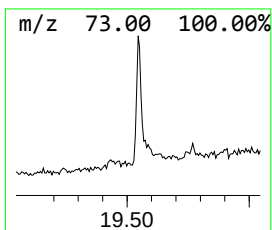
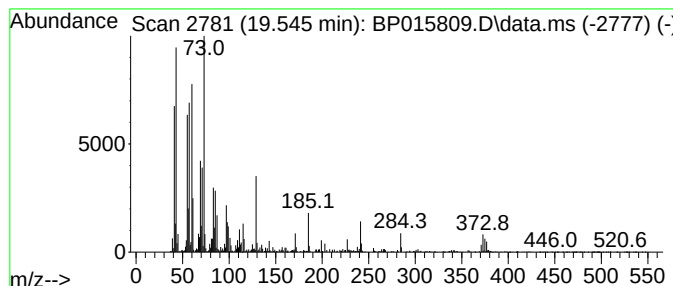
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TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.545	4.00 ng/ul	526635	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	98
4			Octadecanoic acid	284	C18H36O2	000057-11-4	96
5			Octadecanoic acid	284	C18H36O2	000057-11-4	93



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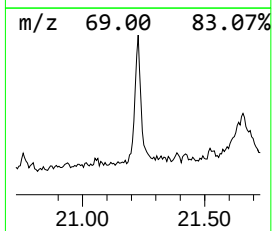
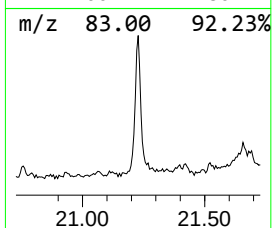
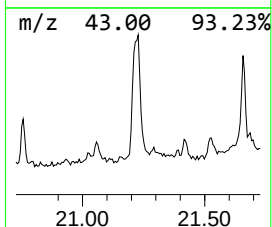
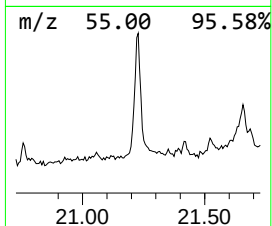
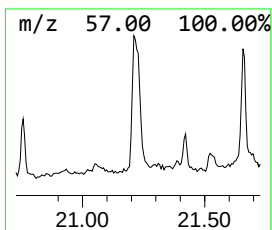
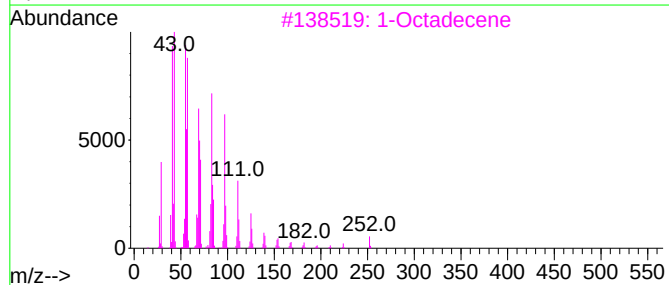
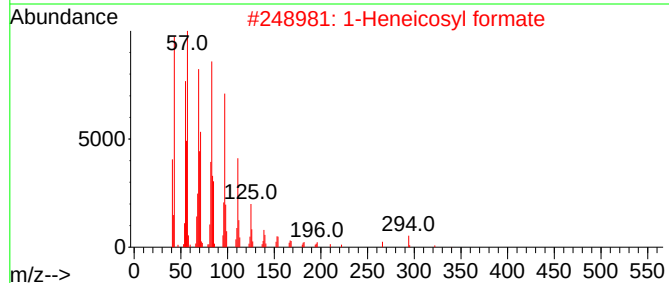
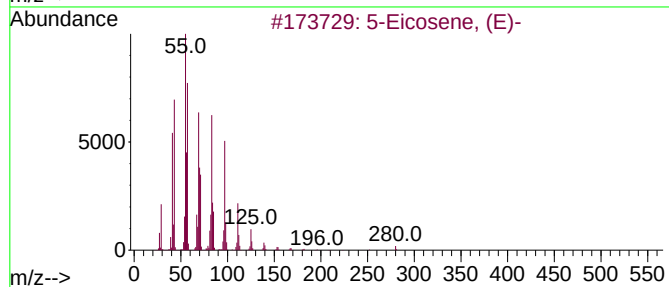
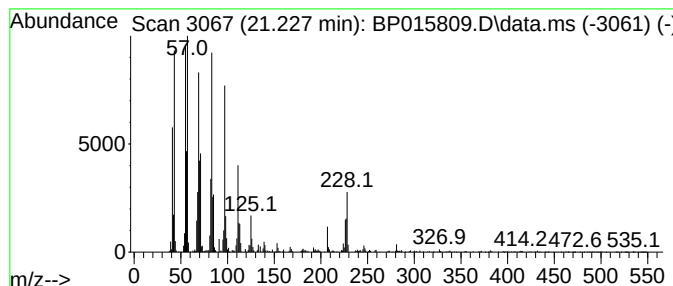
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	7.44 ng/ul	979358	Chrysene-d12	21.557

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	99
2	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94
3	1-Octadecene		252	C18H36	000112-88-9	93
4	1-Octadecanol		270	C18H38O	000112-92-5	93
5	Bromoacetic acid, octadecyl ester		390	C20H39BrO2	018992-03-5	91



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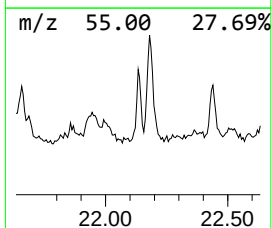
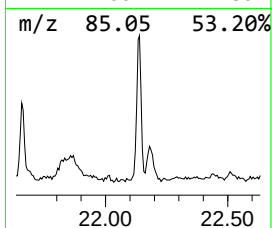
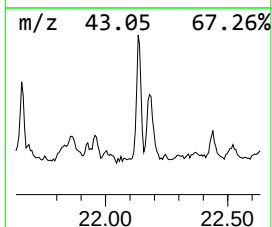
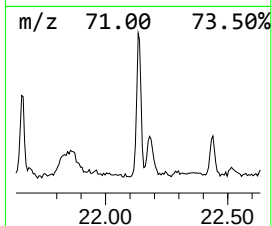
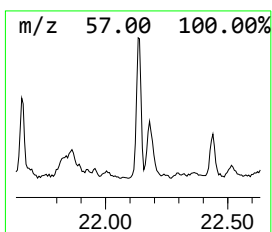
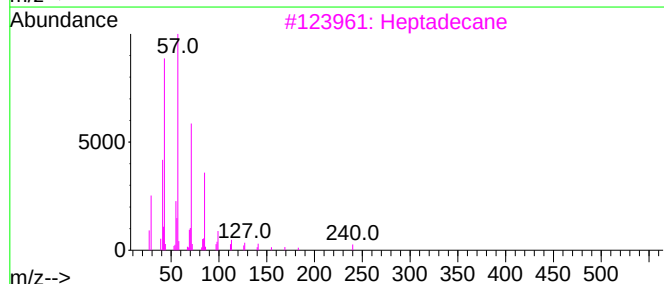
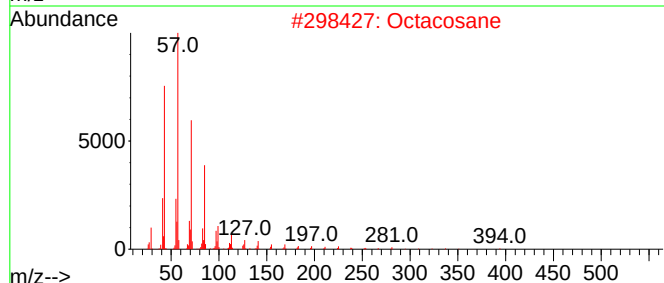
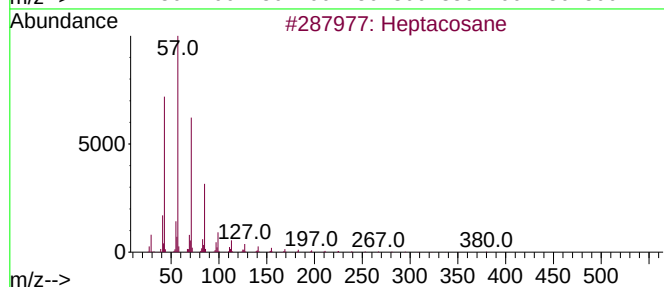
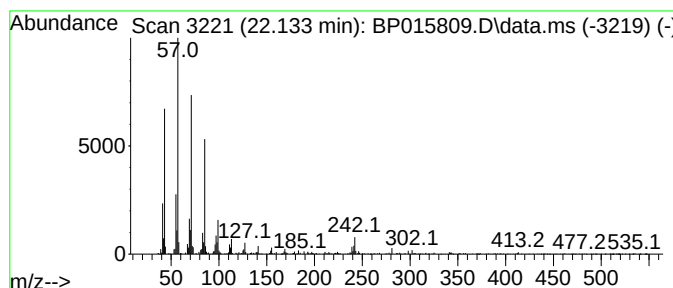
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.133	2.63 ng/ul	345634	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	96
2			Octacosane	394	C28H58	000630-02-4	96
3			Heptadecane	240	C17H36	000629-78-7	94
4			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	90
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
Data File : BP015809.D
Acq On : 29 Jun 2023 14:05
Operator : MA/JU
Sample : 03143-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFV1

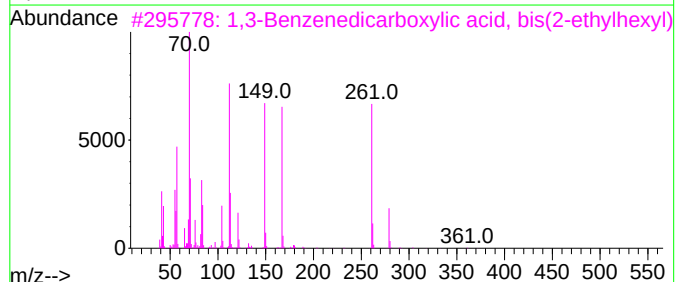
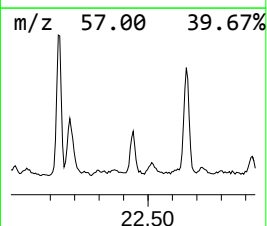
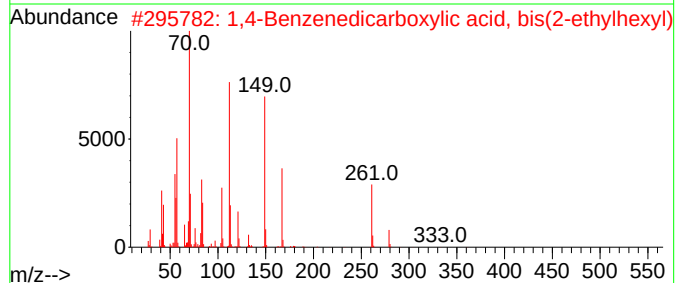
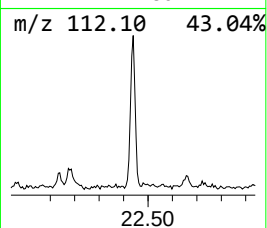
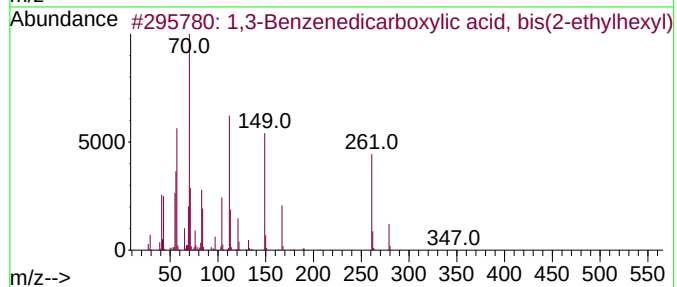
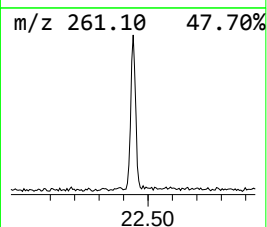
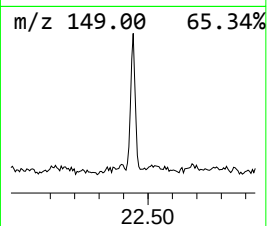
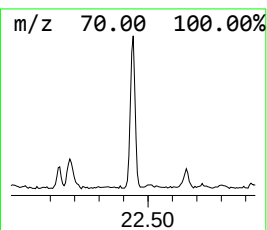
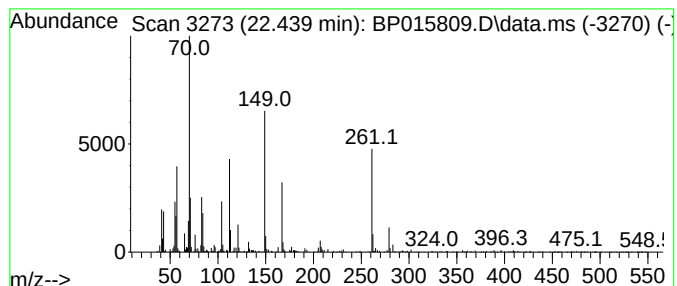
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 1,3-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.439	3.57 ng/ul	470140	Chrysene-d12	21.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	68		
2	1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	59		
3	1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	53		
4	1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	38		
5	1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	38		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
Data File : BP015809.D
Acq On : 29 Jun 2023 14:05
Operator : MA/JU
Sample : 03143-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFV1

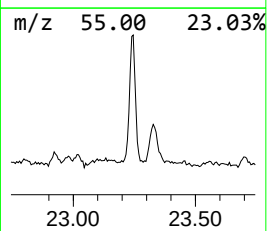
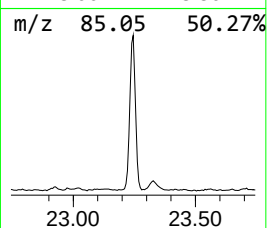
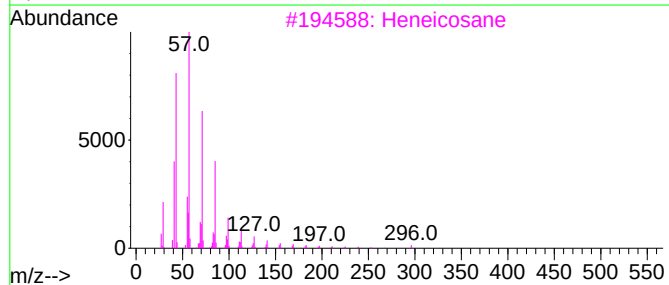
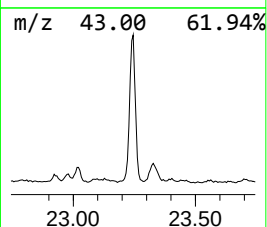
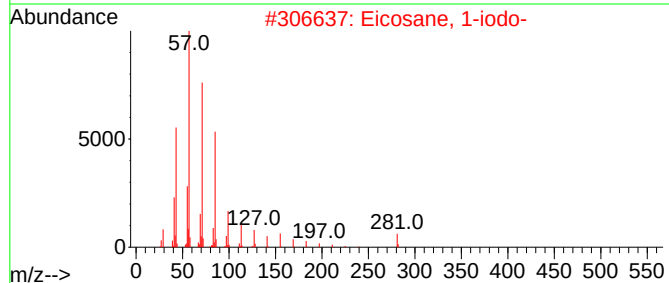
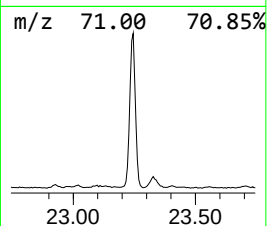
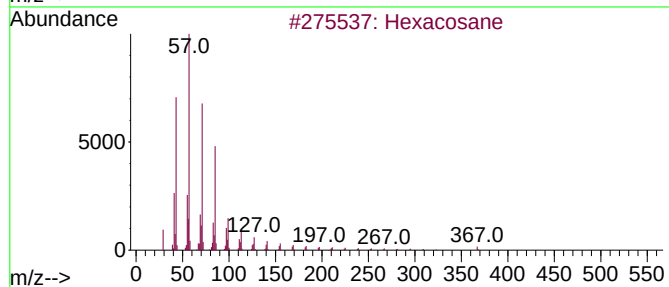
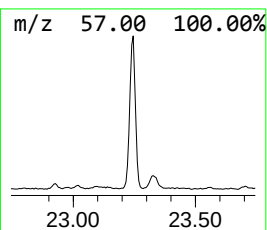
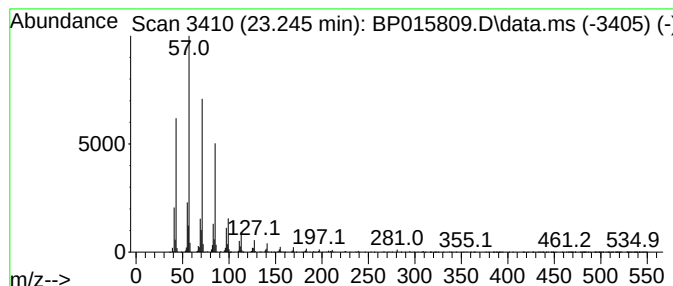
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Quant Title : SVOA CALIBRATION

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.
23.245	15.40 ng/ul	2292490	Perylene-d12	24.104

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91
5			Nonacosane	408	C29H60	000630-03-5	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
Data File : BP015809.D
Acq On : 29 Jun 2023 14:05
Operator : MA/JU
Sample : 03143-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFV1

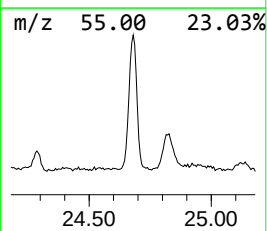
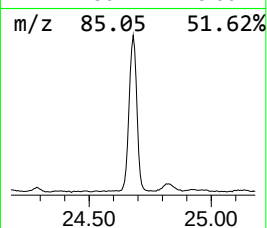
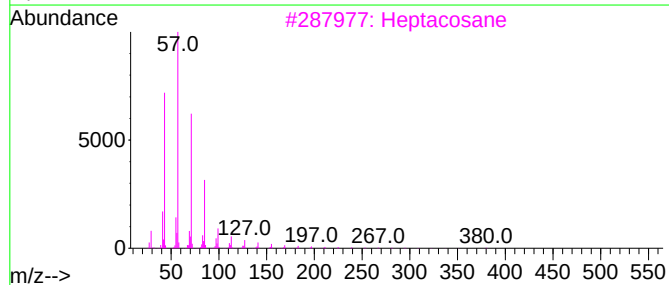
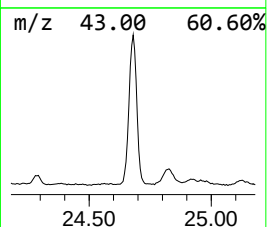
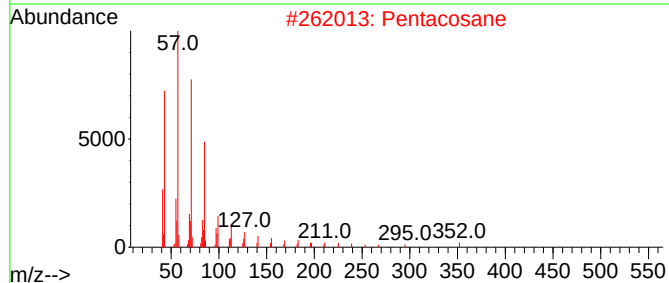
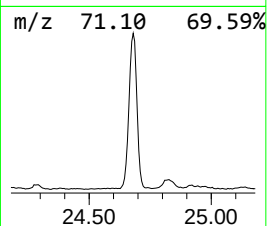
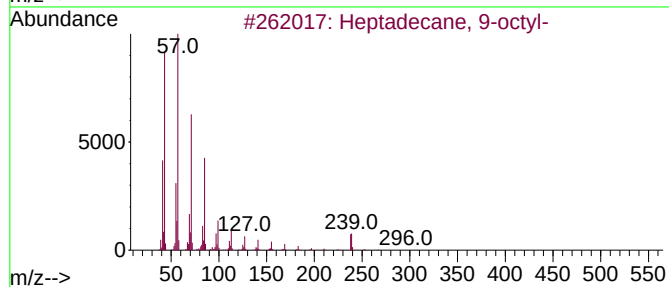
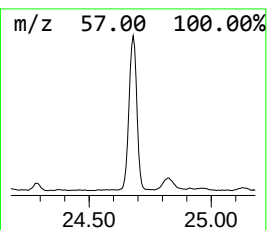
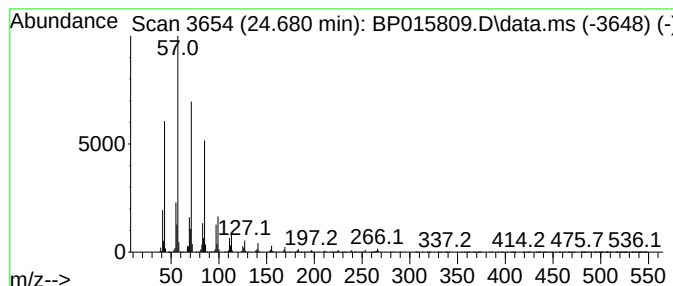
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Quant Title : SVOA CALIBRATION

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.680	25.50 ng/ul	3795530	Perylene-d12	24.104

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2		Pentacosane	352	C25H52	000629-99-2	94
3		Heptacosane	380	C27H56	000593-49-7	93
4		2-Bromo dodecane	248	C12H25Br	013187-99-0	93
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
Data File : BP015809.D
Acq On : 29 Jun 2023 14:05
Operator : MA/JU
Sample : 03143-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

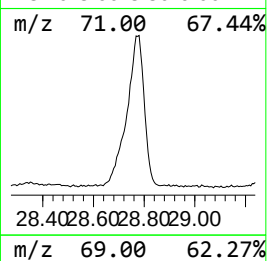
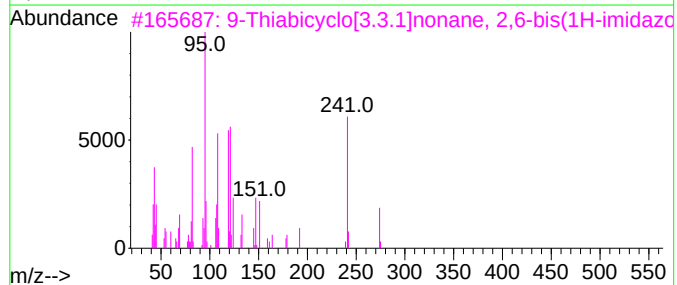
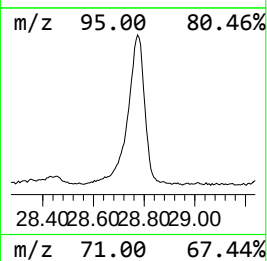
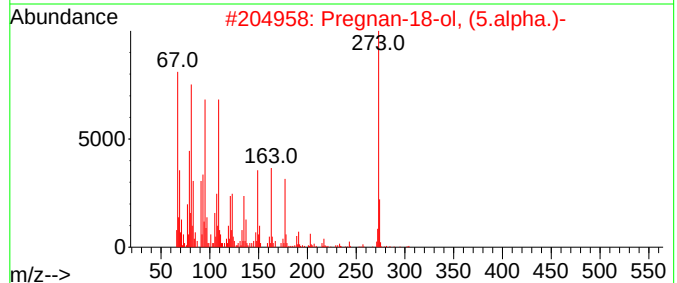
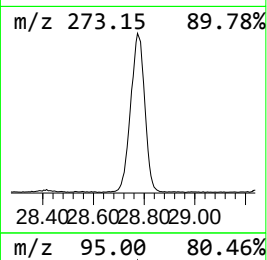
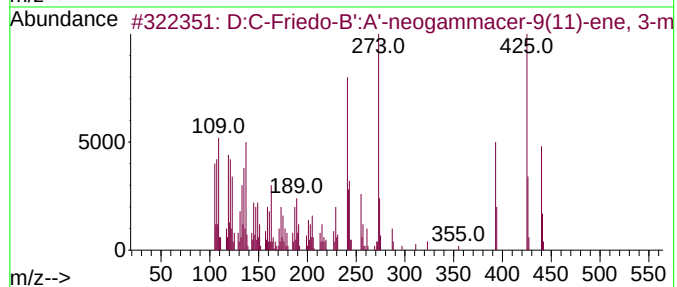
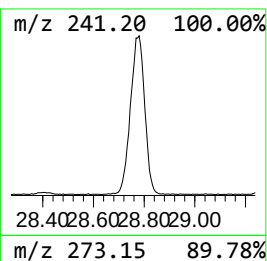
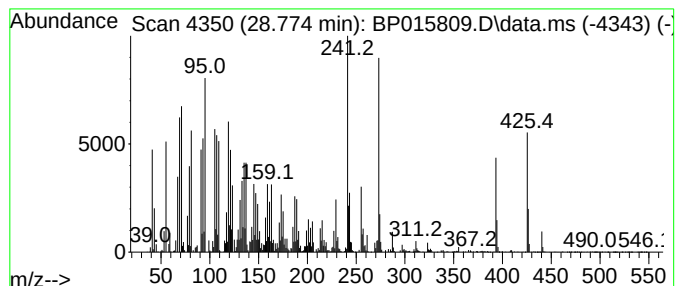
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 9 D:C-Friedo-B':A'-neogammace... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
28.774	72.63 ng/ul	10809200	Perylene-d12			24.104
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...		440	C31H52O	004555-56-0	53
2	Pregnan-18-ol, (5.alpha.)-		304	C21H36O	056053-09-9	46
3	9-Thiabicyclo[3.3.1]nonane, 2,6-...		274	C14H18N4S	1000141-52-1	25
4	5-(2-Butenyl)-17-oxo-4-nor-3,5-s...		360	C23H36O3	1000074-89-7	22
5	[1,2,4]Triazolo[1,5-a]pyrimidin-...		241	C12H11N5O	1000351-09-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP062923\
Data File : BP015809.D
Acq On : 29 Jun 2023 14:05
Operator : MA/JU
Sample : 03143-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCFV1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.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
1,3-Benzenediam...	18.251	3.0	ng/ul	383669	4	17.469	2544050	20.0
n-Hexadecanoic ...	18.322	8.9	ng/ul	1130440	4	17.469	2544050	20.0
Octadecanoic acid	19.545	4.0	ng/ul	526635	5	21.557	2633000	20.0
(DEL) Alkane: S...	21.227	7.4	ng/ul	979358	5	21.557	2633000	20.0
(DEL) Alkane: S...	22.133	2.6	ng/ul	345634	5	21.557	2633000	20.0
1,3-Benzenedica...	22.439	3.6	ng/ul	470140	5	21.557	2633000	20.0
(DEL) Alkane: S...	23.245	15.4	ng/ul	2292490	6	24.104	2976340	20.0
(DEL) Alkane: S...	24.680	25.5	ng/ul	3795530	6	24.104	2976340	20.0
D:C-Friedo-B':A...	28.774	72.6	ng/ul	10809200	6	24.104	2976340	20.0