LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

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: BP015881.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.375	29	32	40	rVB	66267	91789	0.35%	0.106%
2	3.822	105	108	122	rBV	462687	771553	2.92%	0.893%
3	3.922	122	125	132	rVB	62820	94649	0.36%	0.110%
4	4.040	141	145	151	rVB	60461	96368	0.36%	0.112%
5	7.234	681	688	706	rBV	622220	1546530	5.85%	1.791%
6	7.375	706	712	733	rVB	742079	1368354	5.17%	1.584%
7	7.581	740	747	769	rBV	905959	1694667	6.41%	1.962%
8	8.052	819	827	846	rBV	819173	1562897	5.91%	1.810%
9	8.793	945	953	971	rBV	540932	1392682	5.27%	1.613%
10	9.240	1022	1029	1054	rBV	780916	1670798	6.32%	1.935%
11	9.969	1144	1153	1180	rBV	579870	1386244	5.24%	1.605%
12	10.540	1240	1250	1283	rBV	555400	1910313	7.22%	2.212%
13	10.881	1300	1308	1327	rBV	1134430	2196004	8.30%	2.543%
14	11.057	1329	1338	1367	rBV	362007	1321152	4.99%	1.530%
15	13.581	1761	1767	1772	rBV	30067	52827	0.20%	0.061%
16	13.951	1824	1830	1835	rBV6	32432	54458	0.21%	0.063%
17	14.110	1851	1857	1871	rBV	1591185	2681918	10.14%	3.106%
18	14.398	1898	1906	1921	rBV	2035487	3283294	12.41%	3.802%
19	14.704	1949	1958	1974	rBV	1541204	2513514	9.50%	2.911%
20	15.004	2002	2009	2025	rBV2	161210	662176	2.50%	0.767%
21	15.704	2121	2128	2144	rBV	2050143	3657770	13.83%	4.236%
22	15.875	2152	2157	2179	rVB	197200	556934	2.11%	0.645%
23	16.069	2184	2190	2208	rBV	458513	761404	2.88%	0.882%
24	16.551	2268	2272	2278	rBV5	32656	59931	0.23%	0.069%
25	16.628	2281	2285	2293	rVB2	49921	85719	0.32%	0.099%
26	16.839	2318	2321	2328	rBV8	28679	60227	0.23%	0.070%
27	17.151	2370	2374	2376	rBV3	23280	30539	0.12%	0.035%
28	17.333	2401	2405	2413	rBV	73118	122309	0.46%	0.142%
29	17.404	2413	2417	2421	rBV4	44458	59928	0.23%	0.069%
30	17.463	2421	2427	2433	rBV	1484612	2277944	8.61%	2.638%
31	17.569	2439	2445	2466	rVB2	1766141	3223678	12.19%	3.733%
32	18.204	2551	2553	2558	rVB3	39388	47753	0.18%	0.055%
33	18.263	2558	2563	2567	rBV	196586	284249	1.07%	0.329%
34	18.316	2567	2572	2581	rBV	1296245	1866080	7.06%	2.161%
35	18.892	2667	2670	2675	rVB4	63465	84479	0.32%	0.098%
36	19.404	2754	2757	2759	rBV	74902	92775	0.35%	0.107%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

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

37	19.469	2764	2768	2776	rVB	361475	571511	2.16%	0.662%
38	19.539	2777	2780	2787	rBV	315185	462586	1.75%	0.536%
39	19.792	2818	2823	2836	rBV2	2517641	4045930	15.30%	4.685%
40	21.222	3063	3066	3074	rVB2	673878	1009635	3.82%	1.169%
41	21.551	3117	3122	3127	rBV3	1550119	2593747	9.81%	3.003%
42	23.233	3404	3408	3415	rVB	969076	1534343	5.80%	1.777%
43	23.927	3522	3526	3533	rVB2	1580628	3098556	11.71%	3.588%
44	24.098	3550	3555	3573	rVB	1102270	2563588	9.69%	2.969%
45	24.668	3646	3652	3661	rVB	1053521	2207979	8.35%	2.557%
46	26.627	3979	3985	3993	rVB2	876114	2197559	8.31%	2.545%
47	28.774	4338	4350	4367	rVB3	6283412	26450038	100.00%	30.628%

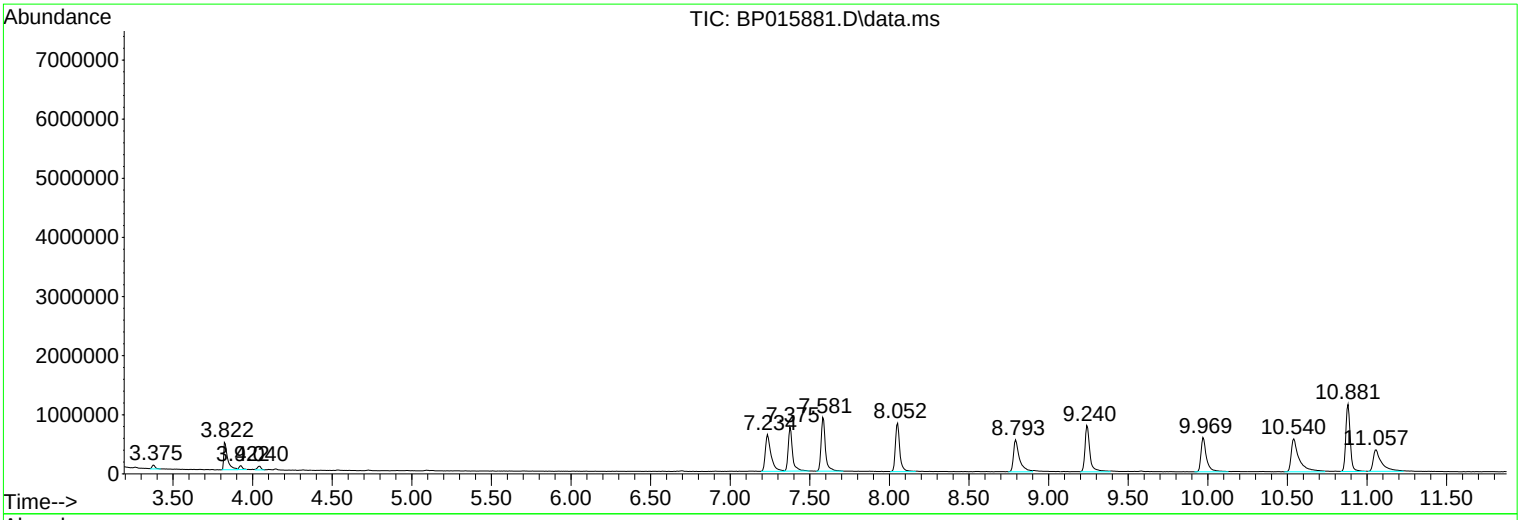
Sum of corrected areas: 86359378

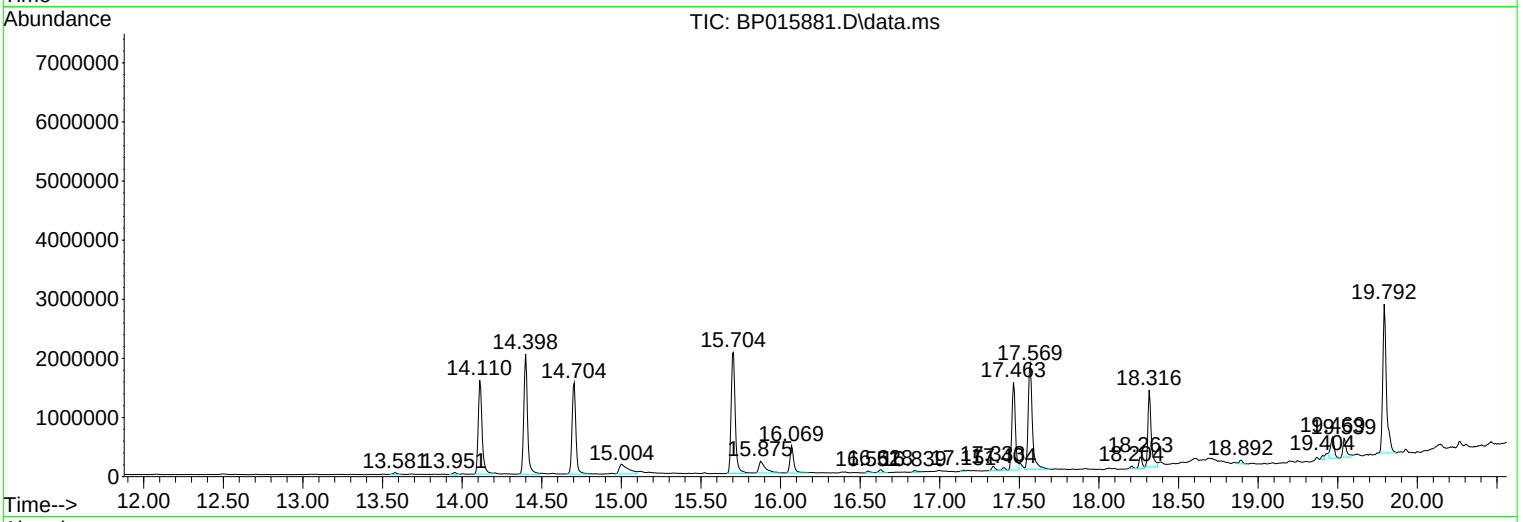
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

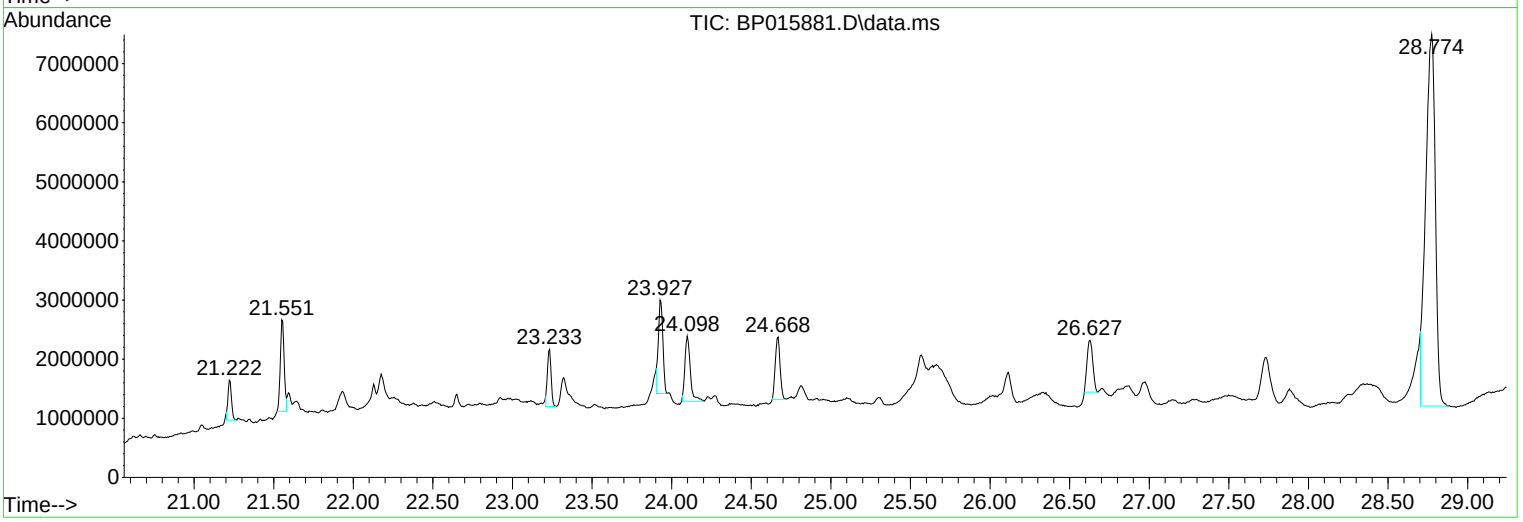
Instrument :
BNA_P
ClientSampleId :
DCGA4

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

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

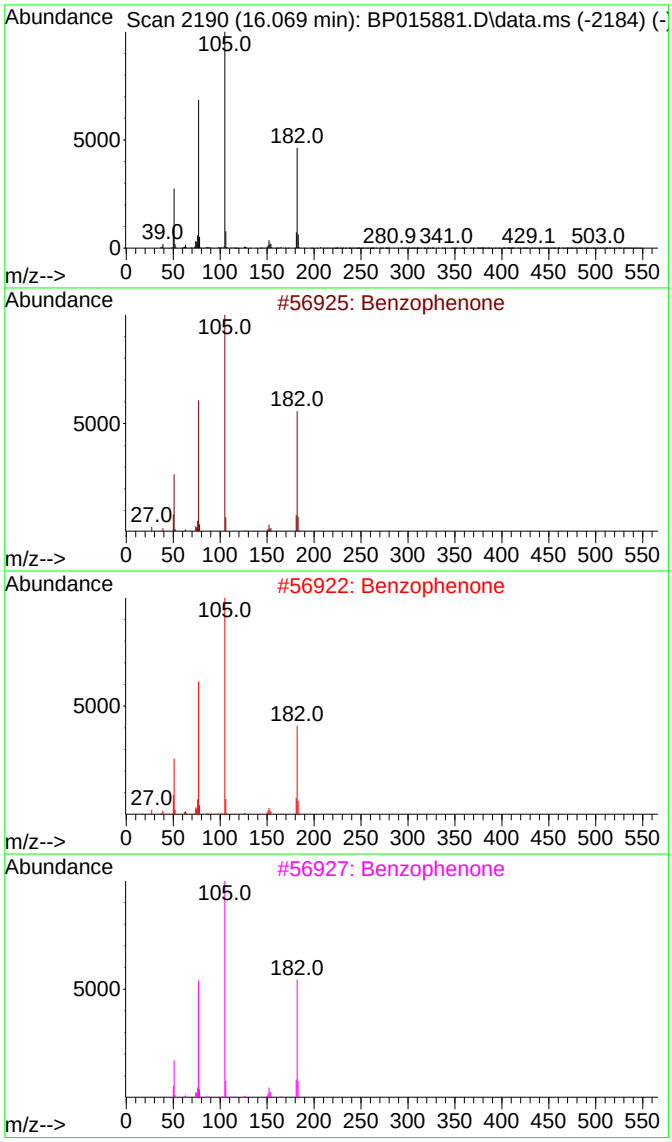
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

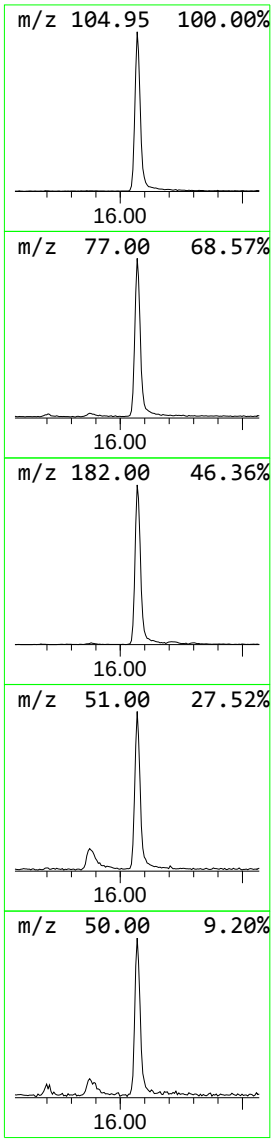
****

Peak Number 1 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.069	6.06 ng/ul	761404	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	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

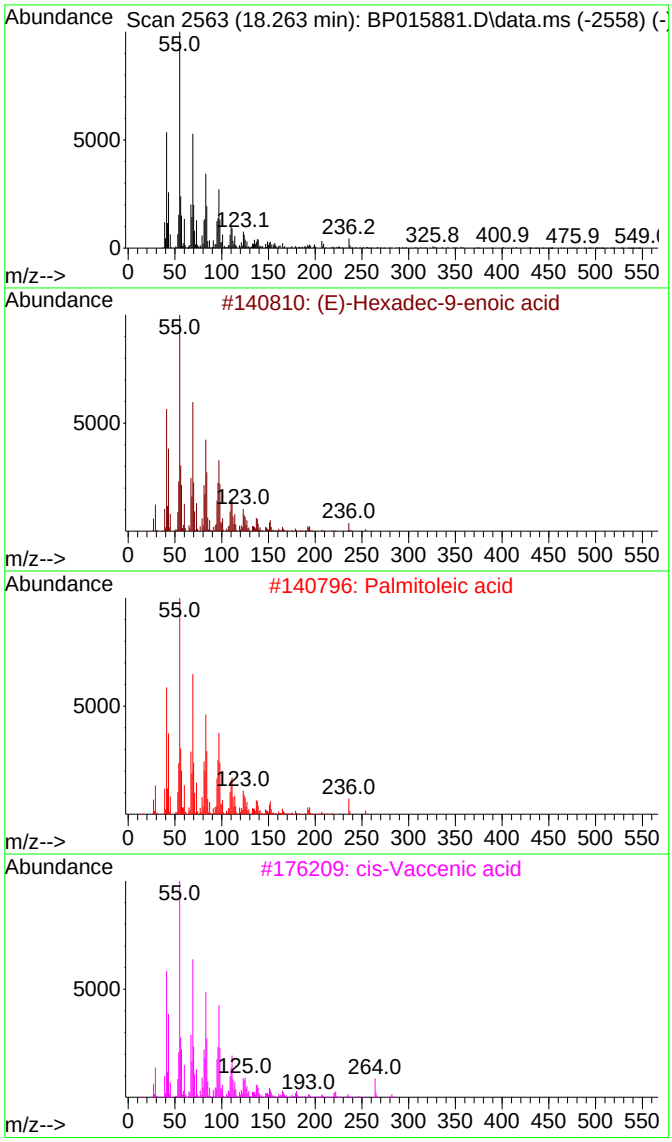
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

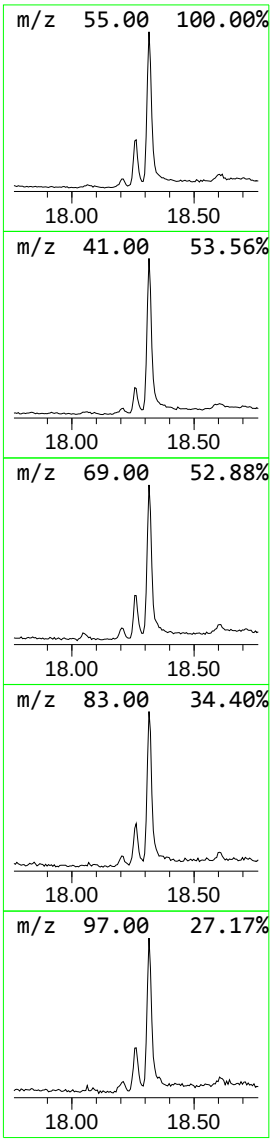
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (E)-Hexadec-9-enoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.263	2.50 ng/ul	284249	Phenanthrene-d10	17.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	94
2	Palmitoleic acid	254	C16H30O2	000373-49-9	91
3	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
4	cis-7-Hexadecenoic acid	254	C16H30O2	002416-19-5	91
5	13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

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

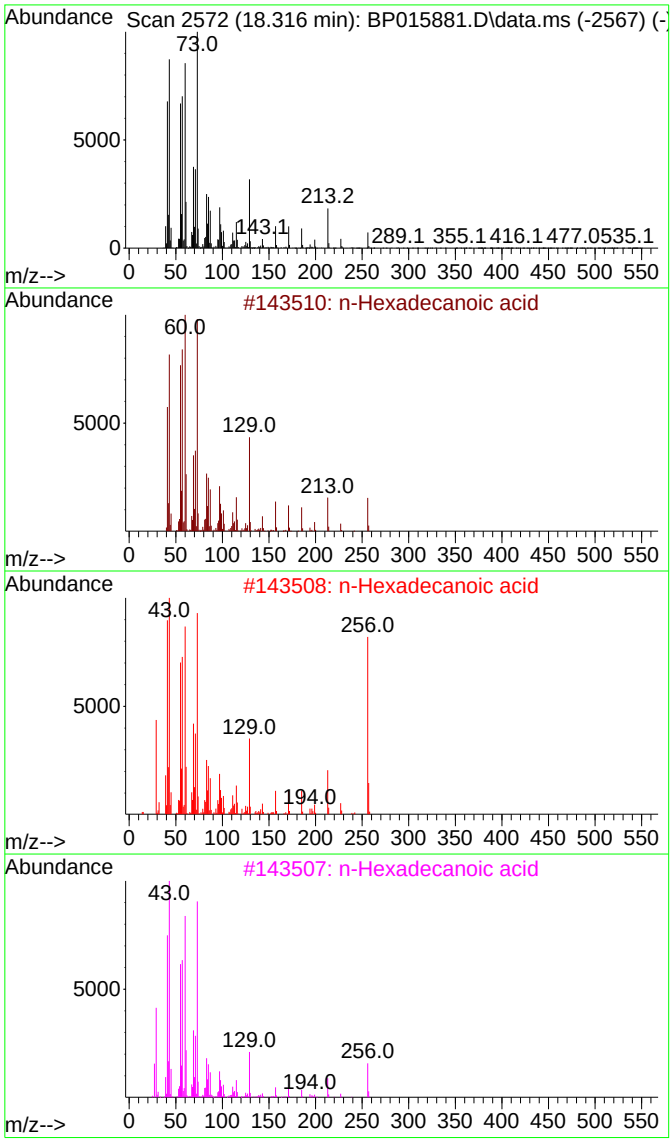
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

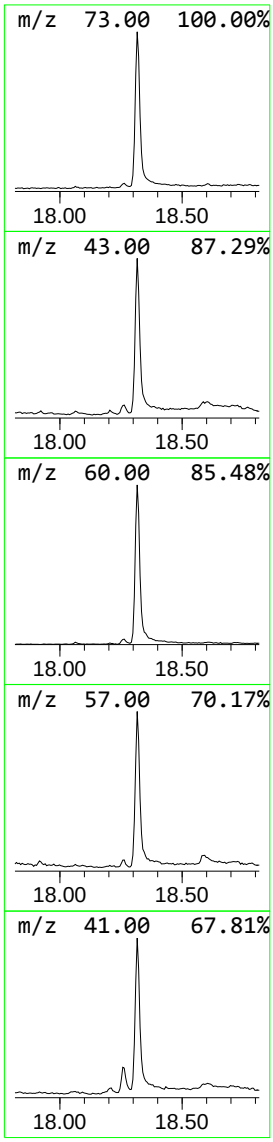
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.316	16.38 ng/ul	1866080	Phenanthrene-d10	17.463

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	97
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

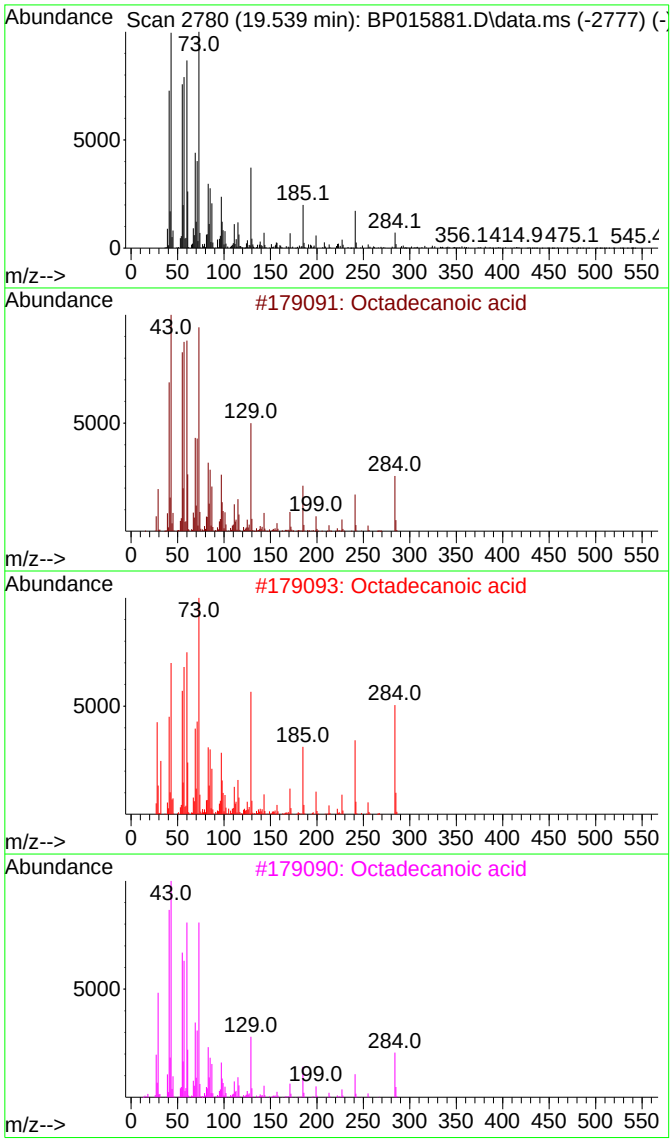
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

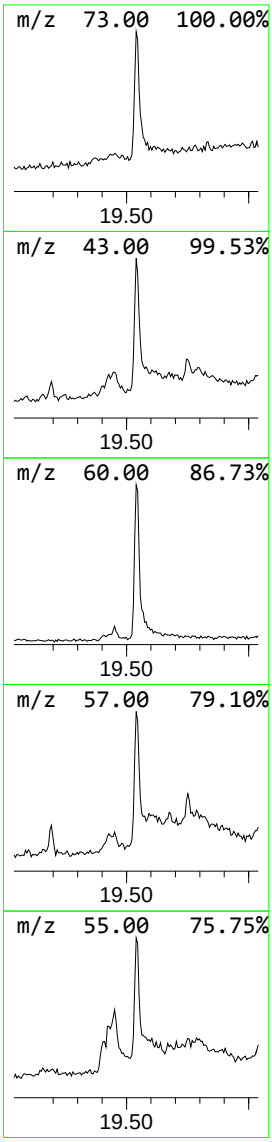
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.539	3.57 ng/ul	462586	Chrysene-d12	21.551

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	97
3	Octadecanoic acid	284	C18H36O2	000057-11-4	96
4	Octadecanoic acid	284	C18H36O2	000057-11-4	94
5	Octadecanoic acid	284	C18H36O2	000057-11-4	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

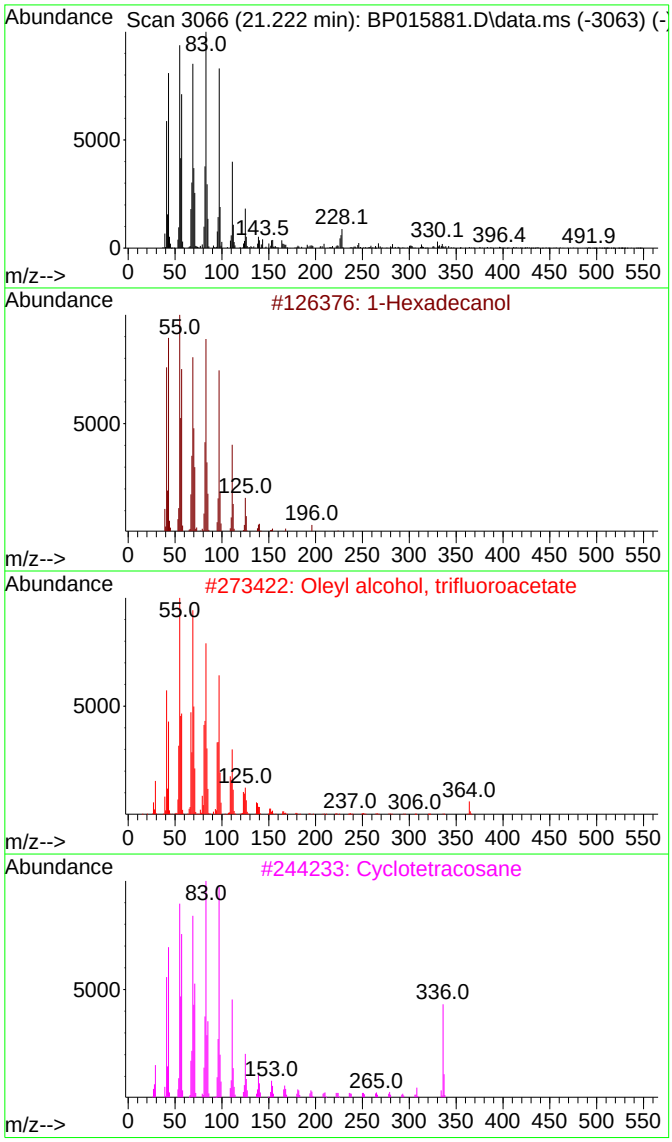
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

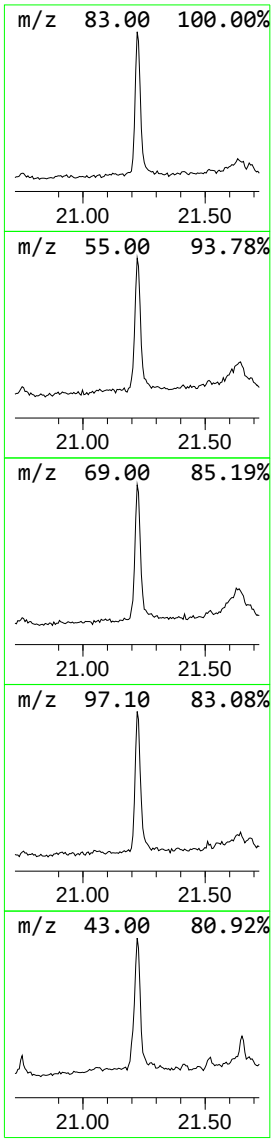
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.221	7.79 ng/ul	1009640	Chrysene-d12	21.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	94
2	Oleyl alcohol, trifluoroacetate	364	C20H35F3O2	1000352-68-4	91
3	Cyclotetracosane	336	C24H48	000297-03-0	91
4	Cyclohexadecane	224	C16H32	000295-65-8	91
5	Heptacos-1-ene	378	C27H54	015306-27-1	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

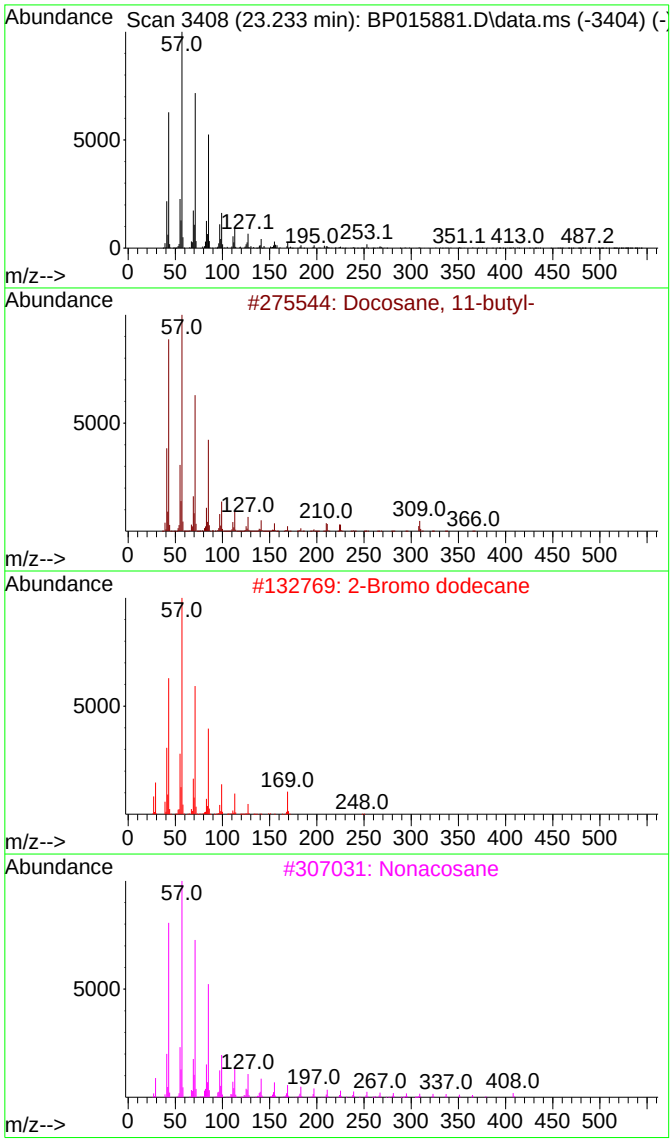
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

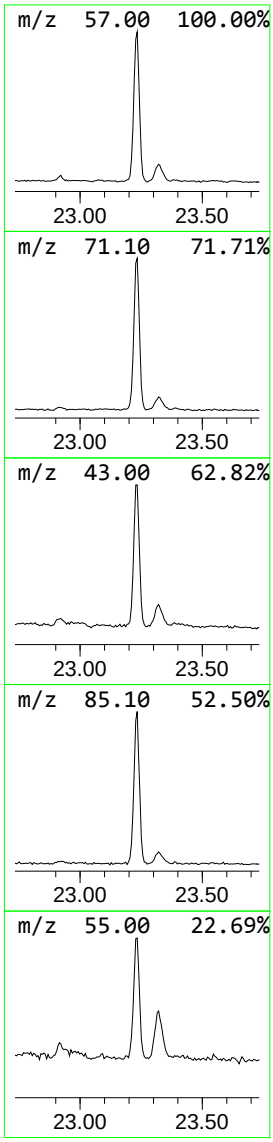
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.233	11.97 ng/ul	1534340	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3	Nonacosane	408	C29H60	000630-03-5	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Docosane, 9-butyl-	366	C26H54	055282-14-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

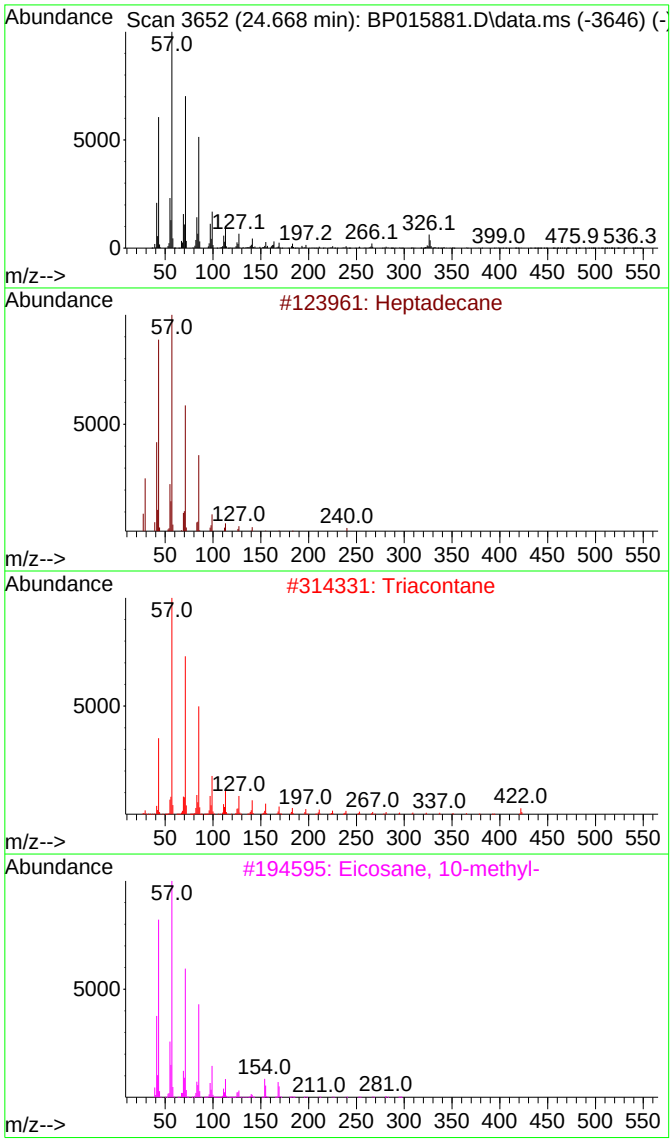
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

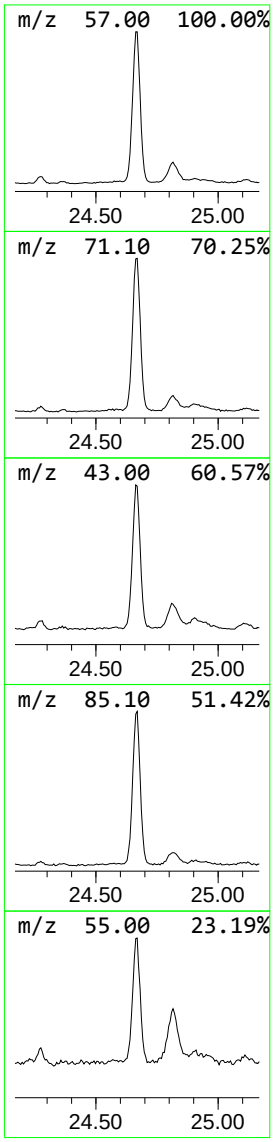
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.668	17.23 ng/ul	2207980	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Triacontane	422	C30H62	000638-68-6	93
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

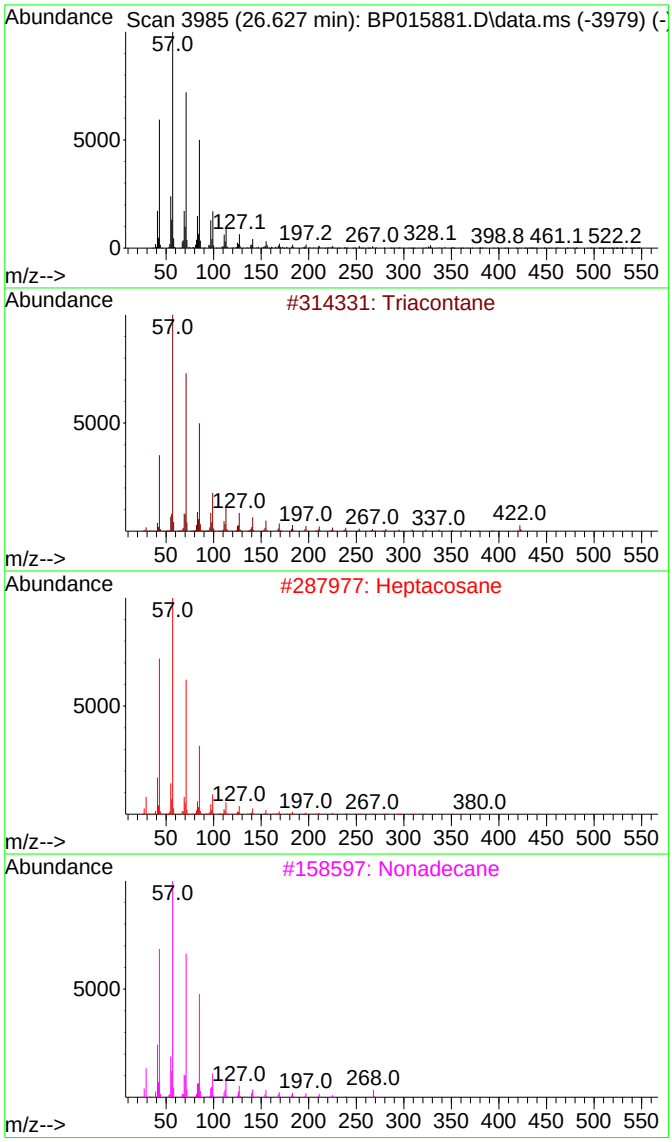
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

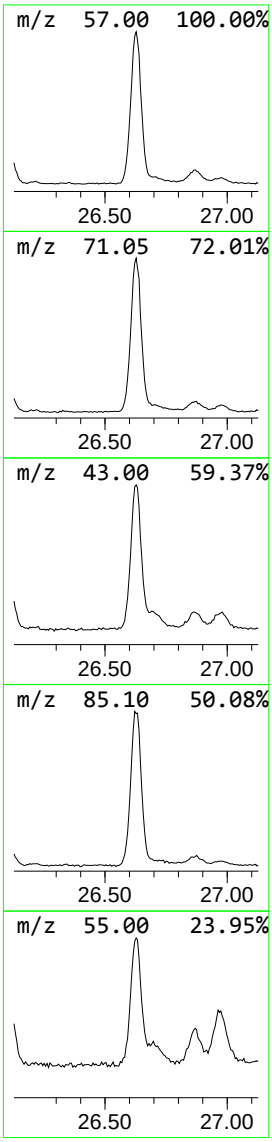
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.627	17.14 ng/ul	2197560	Perylene-d12	24.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	96
2	Heptacosane	380	C27H56	000593-49-7	95
3	Nonadecane	268	C19H40	000629-92-5	94
4	Tricosane	324	C23H48	000638-67-5	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

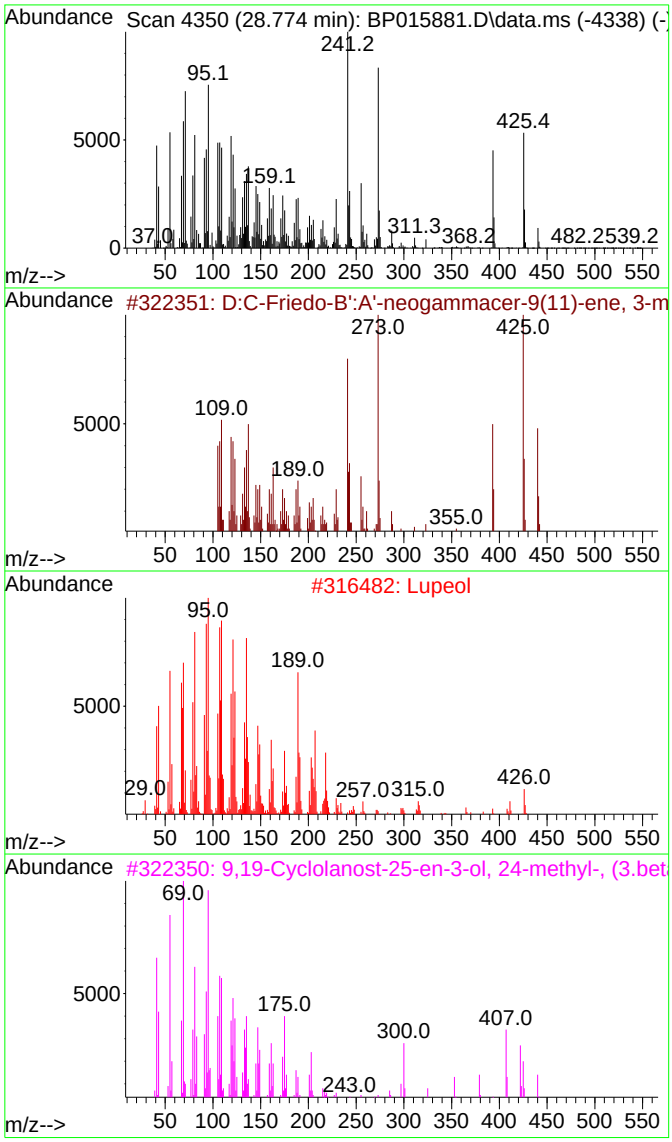
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP062623.MA.M
Quant Title : SVOA CALIBRATION

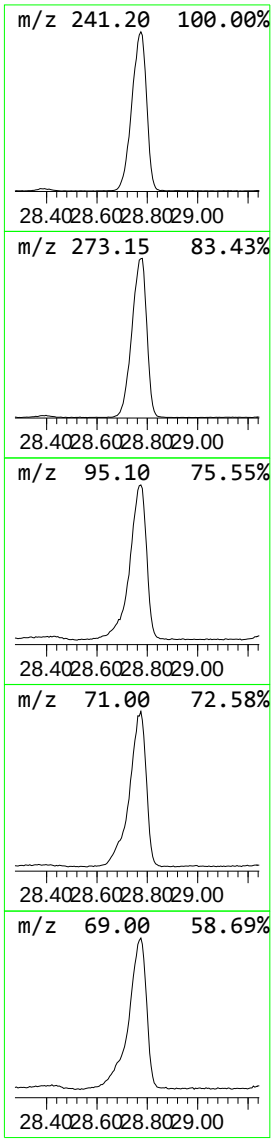
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.774	206.35 ng/ul	26450000	Perylene-d12	24.098

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	Lupeol	426	C30H50O	000545-47-1	53
3	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	42
4	1-(3-Fluoro-phenyl)-4,6-dimethyl...	242	C14H11FN2O	1000300-21-8	22
5	Lupeol	426	C30H50O	000545-47-1	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP063023\
Data File : BP015881.D
Acq On : 01 Jul 2023 12:36
Operator : MA/JU
Sample : 03242-06
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DCGA4

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzophenone	16.069	6.1	ng/ul	761404	3	14.704	2513510	20.0
(E)-Hexadec-9-e...	18.263	2.5	ng/ul	284249	4	17.463	2277940	20.0
n-Hexadecanoic ...	18.316	16.4	ng/ul	1866080	4	17.463	2277940	20.0
Octadecanoic acid	19.539	3.6	ng/ul	462586	5	21.551	2593750	20.0
1-Hexadecanol	21.221	7.8	ng/ul	1009640	5	21.551	2593750	20.0
(DEL) Alkane: S...	23.233	12.0	ng/ul	1534340	6	24.098	2563590	20.0
(DEL) Alkane: S...	24.668	17.2	ng/ul	2207980	6	24.098	2563590	20.0
(DEL) Alkane: S...	26.627	17.1	ng/ul	2197560	6	24.098	2563590	20.0
D:C-Friedo-B':A...	28.774	206.3	ng/ul	26450000	6	24.098	2563590	20.0