LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM070621\
Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

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_M\METHODS\SFAM-EPA-BM070621.M
Title : SVOA CALIBRATION

Signal : TIC: BM030851.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.258	25	29	37	rBV	26983	36313	0.31%	0.069%
2	3.675	97	100	121	rBV	224655	468831	3.99%	0.895%
3	6.928	646	653	669	rBV	389599	647360	5.51%	1.236%
4	7.098	675	682	694	rBV	295521	475897	4.05%	0.909%
5	7.298	708	716	726	rBV	412705	684086	5.82%	1.307%
6	7.763	788	795	803	rBV	361737	573303	4.88%	1.095%
7	8.463	907	914	927	rBV	441259	713160	6.07%	1.362%
8	8.916	983	991	1002	rBV	328161	563169	4.79%	1.076%
9	9.634	1107	1113	1126	rBV	259994	452110	3.85%	0.864%
10	10.169	1197	1204	1216	rBV	385561	701247	5.97%	1.339%
11	10.357	1231	1236	1253	rBV	24158	71918	0.61%	0.137%
12	10.545	1261	1268	1278	rVB	460439	758245	6.45%	1.448%
13	10.686	1284	1292	1314	rBV	339347	668467	5.69%	1.277%
14	13.804	1816	1822	1838	rBV	562162	826997	7.03%	1.580%
15	14.086	1860	1870	1881	rBV	727702	1096107	9.32%	2.094%
16	14.392	1915	1922	1931	rBV	607484	885026	7.53%	1.690%
17	14.598	1949	1957	1980	rBV	201382	479690	4.08%	0.916%
18	15.386	2084	2091	2100	rBV	867283	1296182	11.03%	2.476%
19	15.510	2107	2112	2128	rBV	226623	350182	2.98%	0.669%
20	15.621	2128	2131	2140	rVB3	10977	16365	0.14%	0.031%
21	16.533	2278	2286	2293	rBV6	8056	24985	0.21%	0.048%
22	17.004	2361	2366	2370	rBV	20823	26035	0.22%	0.050%
23	17.133	2381	2388	2396	rBV	640426	921363	7.84%	1.760%
24	17.227	2396	2404	2415	rVV	968018	1426332	12.13%	2.724%
25	17.898	2514	2518	2522	rBV6	6680	12128	0.10%	0.023%
26	18.021	2534	2539	2550	rBV	104311	168870	1.44%	0.323%
27	18.445	2607	2611	2614	rBV2	13629	19412	0.17%	0.037%
28	19.156	2728	2732	2735	rBV	16832	22973	0.20%	0.044%
29	19.304	2753	2757	2764	rVB3	31968	46779	0.40%	0.089%
30	19.404	2771	2774	2779	rBV	10824	15022	0.13%	0.029%
31	19.521	2788	2794	2802	rBV	1794126	2306576	19.62%	4.405%
32	20.515	2958	2963	2968	rBV	248995	286300	2.44%	0.547%
33	20.915	3027	3031	3036	rBV3	52155	68856	0.59%	0.132%
34	21.009	3043	3047	3056	rBV	196665	288544	2.45%	0.551%
35	21.162	3069	3073	3078	rVB	306085	354619	3.02%	0.677%
36	21.245	3083	3087	3092	rBV	612719	749307	6.37%	1.431%

LSC Area Percent Report

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Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

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_M\METHODS\SFAM-EPA-BM070621.M
Title : SVOA CALIBRATION

37	21.303	3092	3097	3106	rVB	758592	1010343	8.59%	1.930%
38	21.727	3166	3169	3174	rVB	93620	117214	1.00%	0.224%
39	21.897	3195	3198	3210	rVB3	85813	139246	1.18%	0.266%
40	22.474	3293	3296	3303	rVB	121861	158551	1.35%	0.303%
41	23.409	3448	3455	3467	rVB	1779479	3391230	28.85%	6.477%
42	23.550	3473	3479	3488	rVB2	590978	1124309	9.56%	2.147%
43	24.644	3656	3665	3675	rVB	1836959	4030136	34.28%	7.697%
44	24.844	3692	3699	3711	rVB5	262941	738631	6.28%	1.411%
45	27.556	4146	4160	4174	rVB	3380461	11388836	96.88%	21.752%
46	27.921	4208	4222	4240	rBV2	3337119	11755913	100.00%	22.453%

Sum of corrected areas: 52357165

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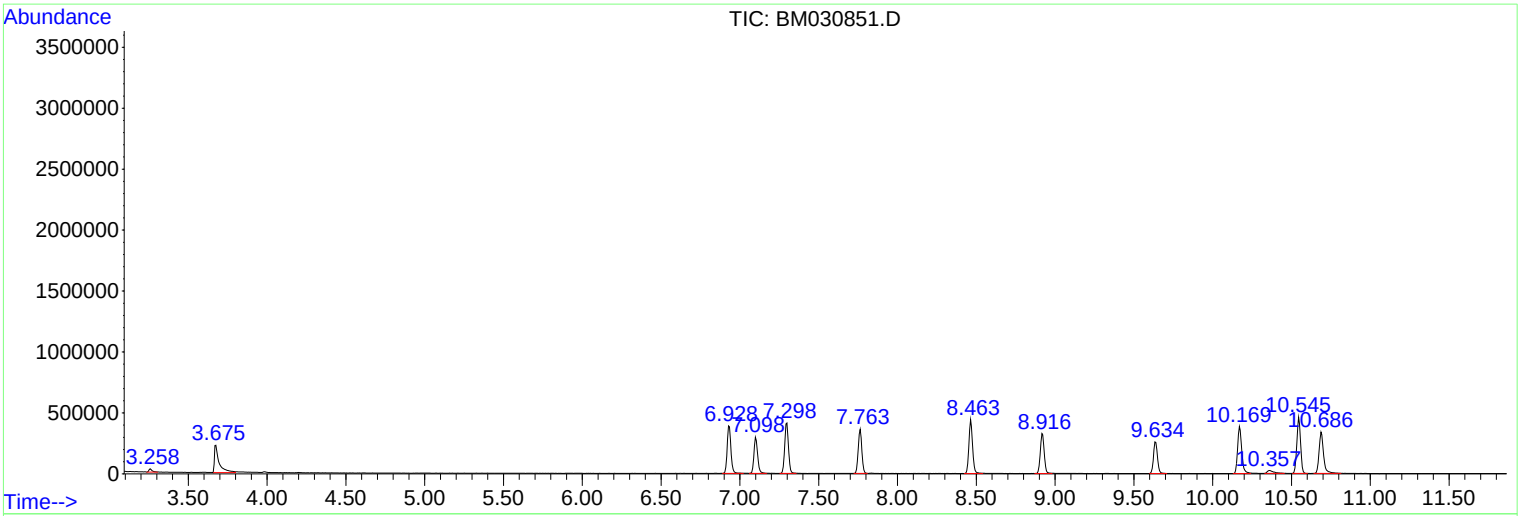
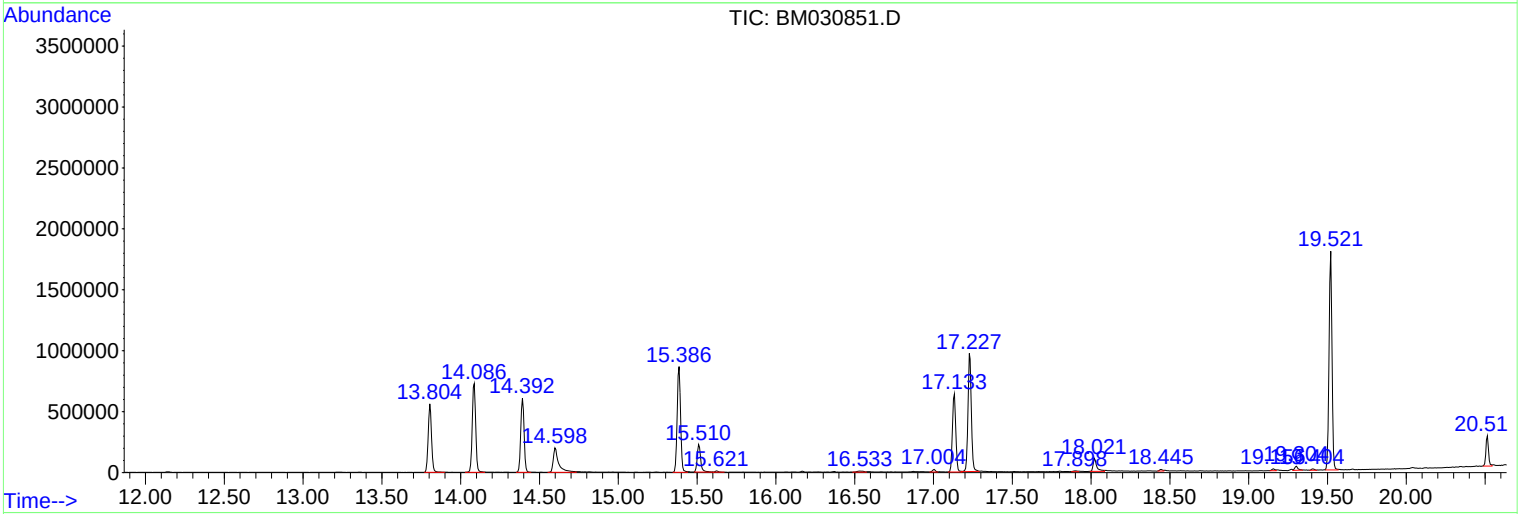
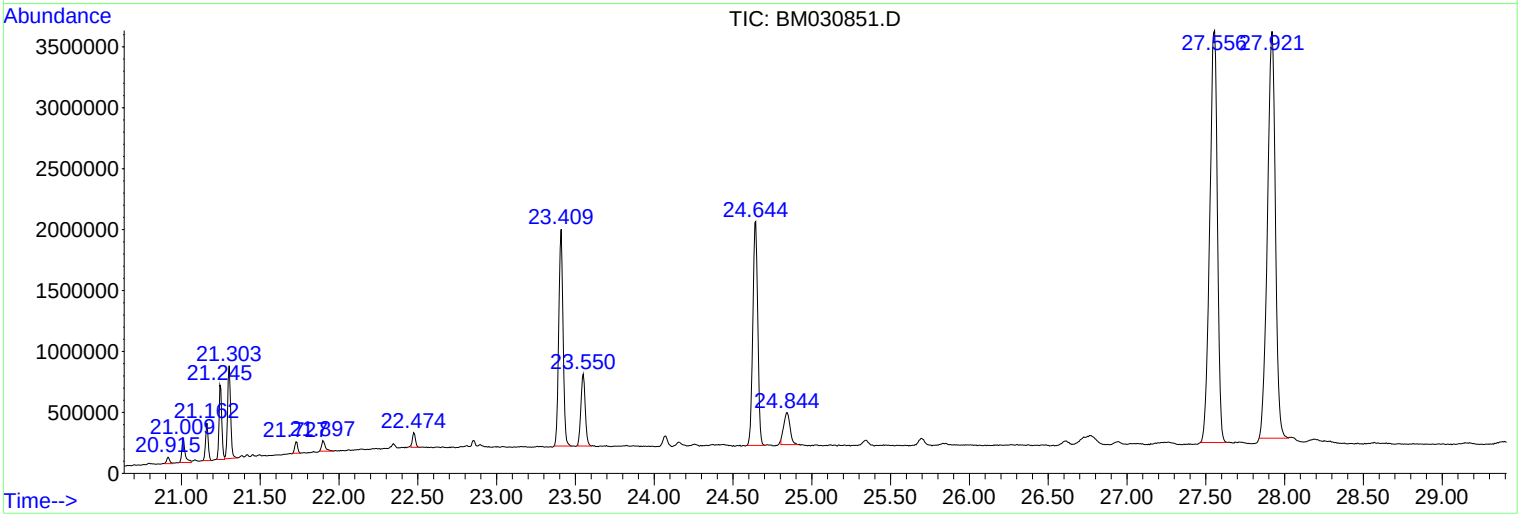
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

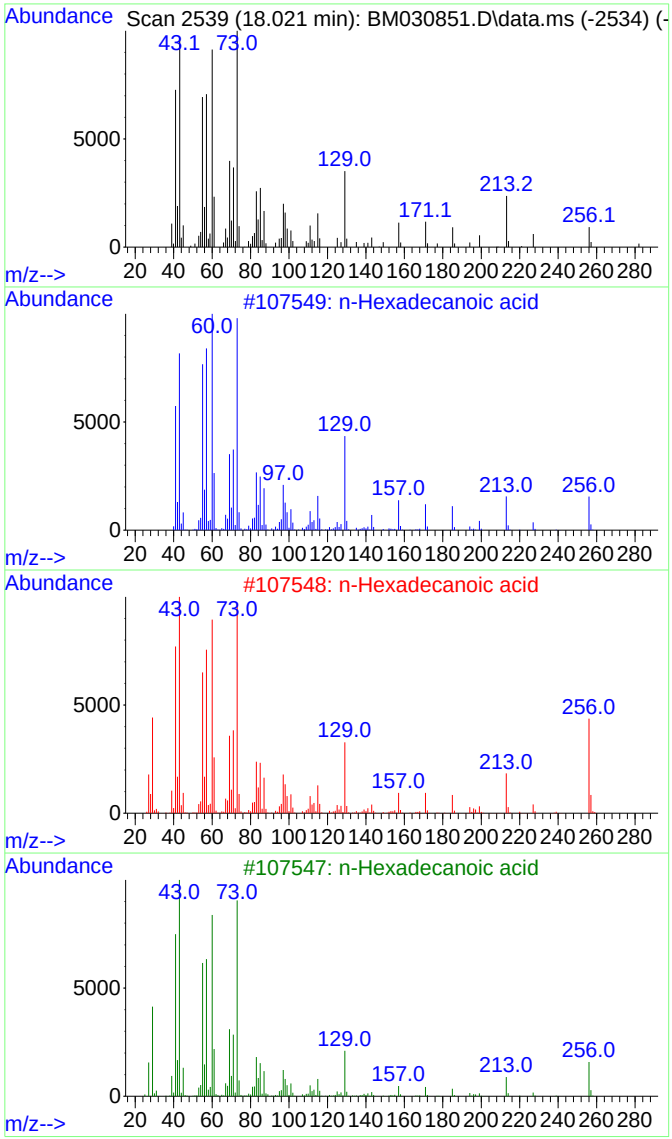
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

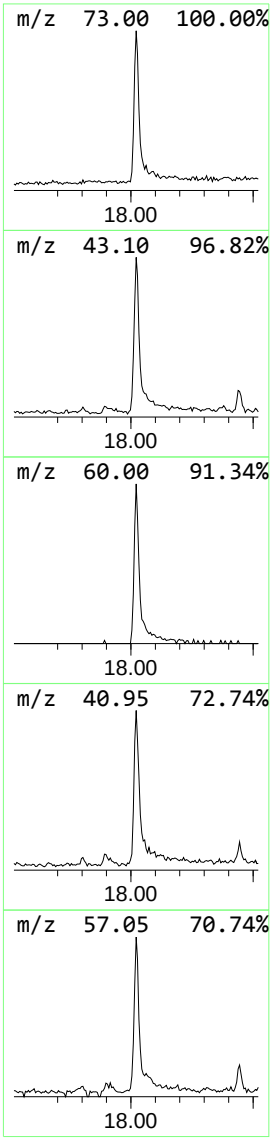
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.020	3.67 ng/ul	168870	Phenanthrene-d10	17.133

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	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72





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Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGDS1

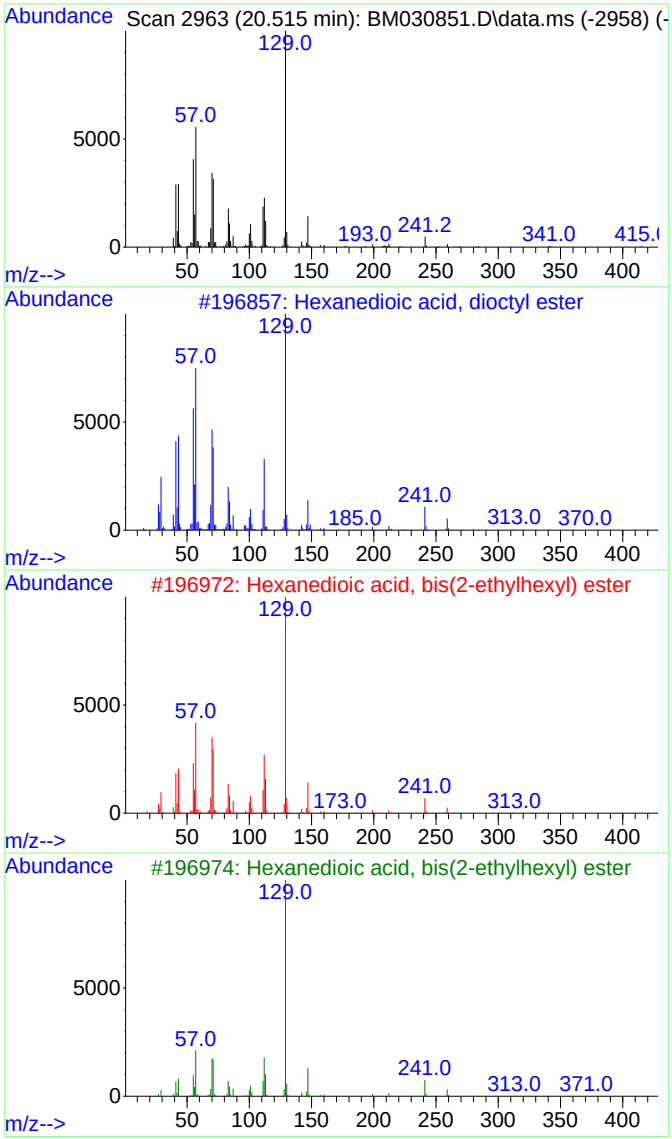
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

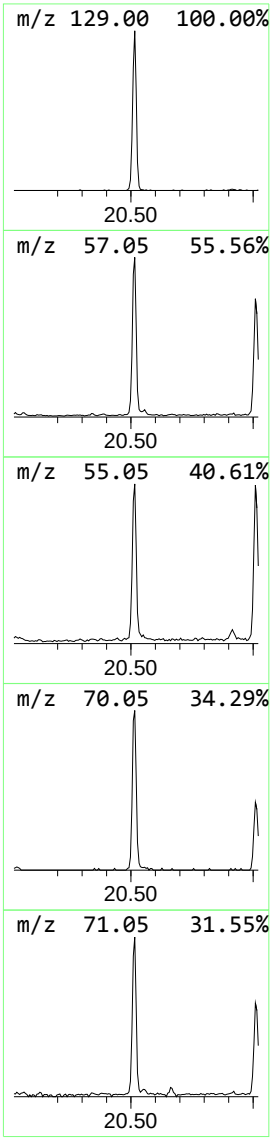
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexanedioic acid, dioctyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.520	5.67 ng/ul	286300	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	90
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
3	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
4	Diisooctyl adipate	370	C22H42O4	001330-86-5	87
5	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	78





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Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

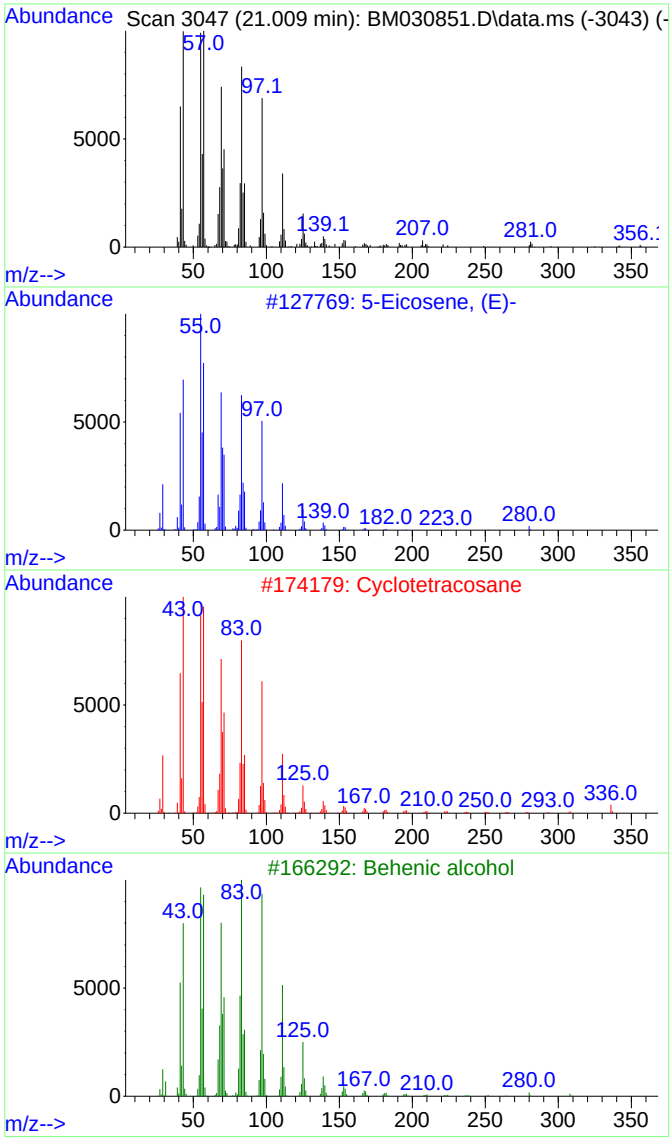
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

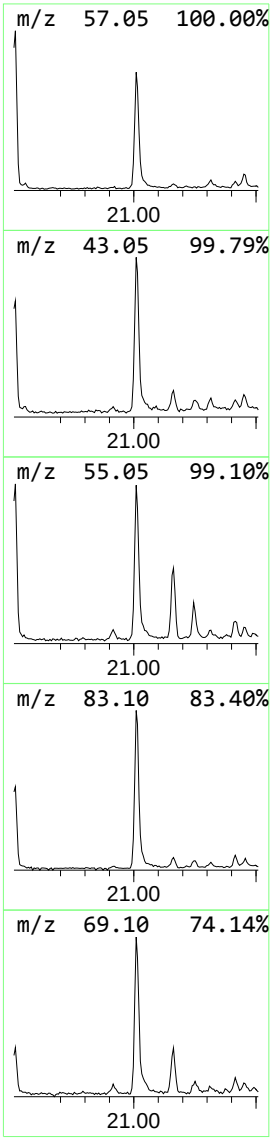
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	5.71 ng/ul	288544	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Cyclotetracosane	336	C24H48	000297-03-0	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

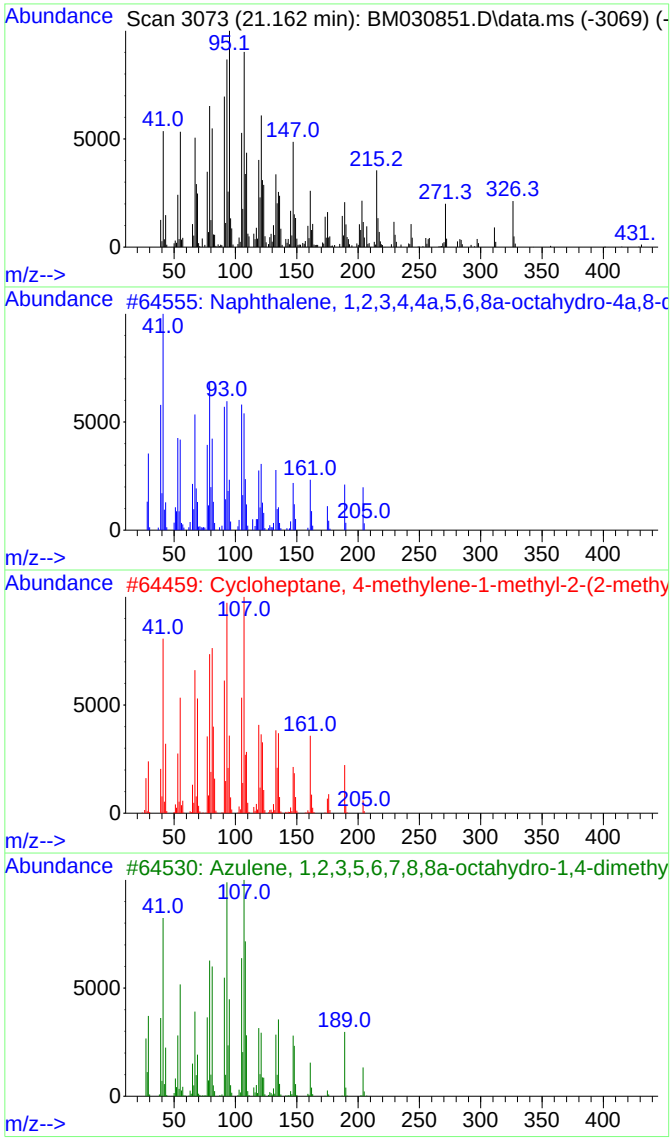
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

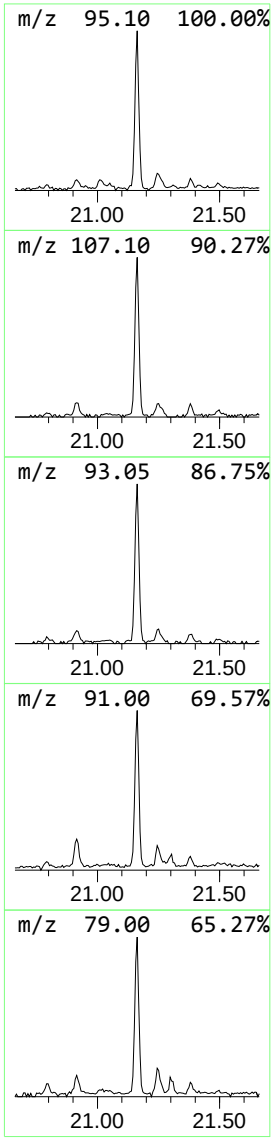
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Naphthalene, 1,2,3,4,4a,5,6... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.160	7.02 ng/ul	354619	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	70
2	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	60
3	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	58
4	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	55
5	.alpha.-Bulnesene	204	C15H24	1000374-19-9	50





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ALS Vial : 28 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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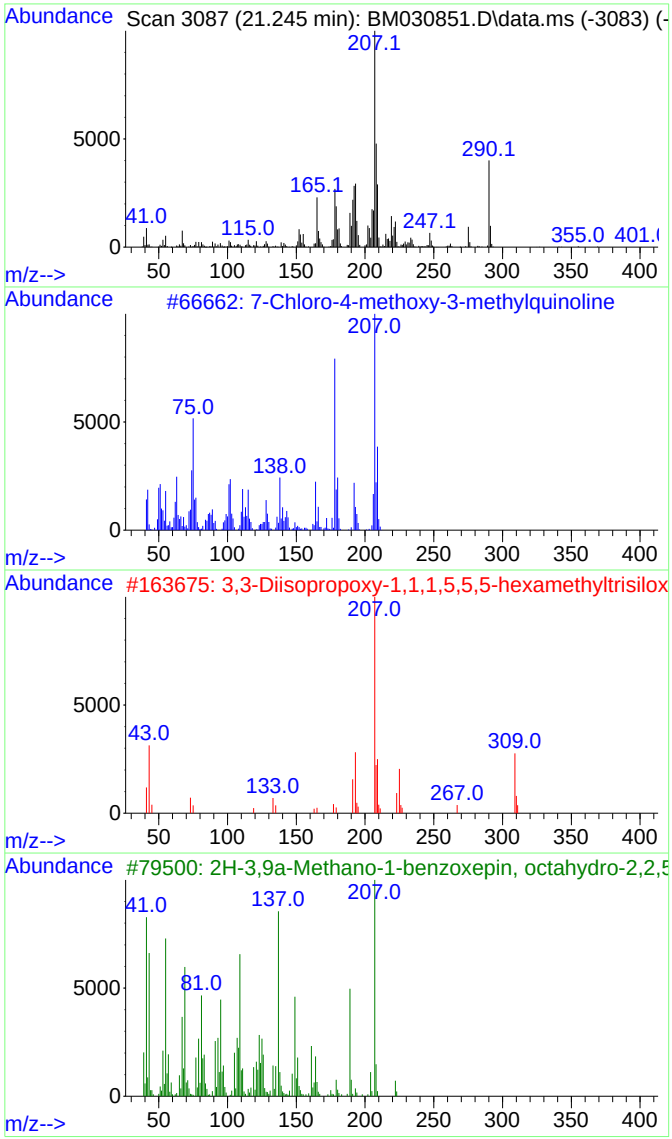
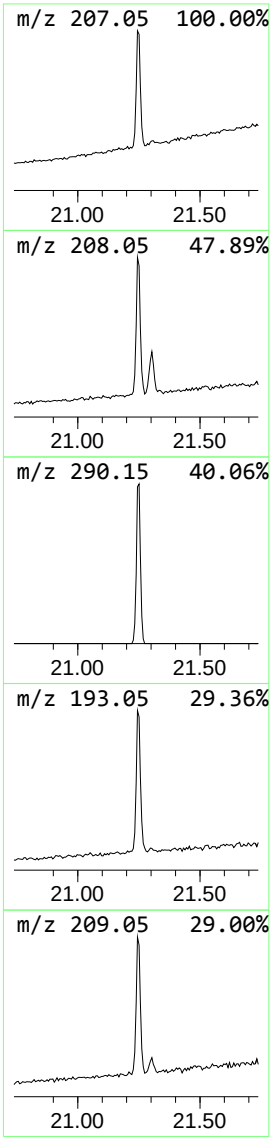
****

Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.240	14.83 ng/ul	749307	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Chloro-4-methoxy-3-methylquino...	207	C11H10ClNO	1000213-52-2	38
2	3,3-Diisopropoxy-1,1,1,5,5,5-hex...	324	C12H32O4Si3	018082-56-9	38
3	2H-3,9a-Methano-1-benzoxepin, oc...	222	C15H26O	005956-09-2	30
4	Thieno[2,3-c]furan-3-carbonitril...	222	C11H14N2OS	447412-24-0	27
5	1-Methyl-3-phenylindole	207	C15H13N	030020-98-5	27





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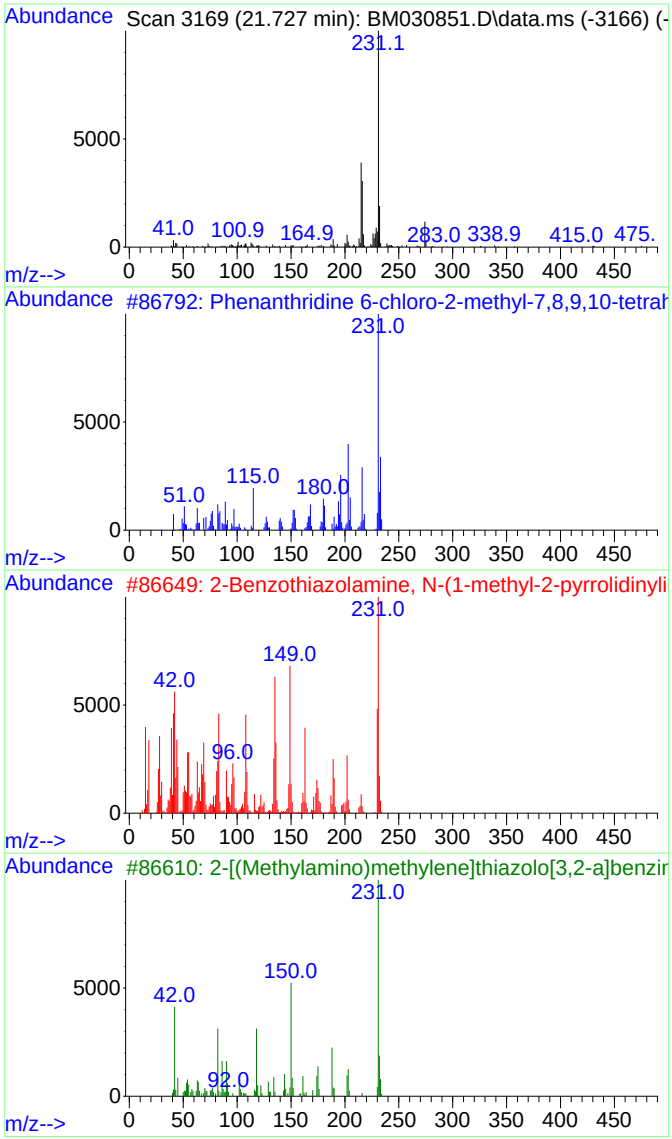
Quant Title : SVOA CALIBRATION

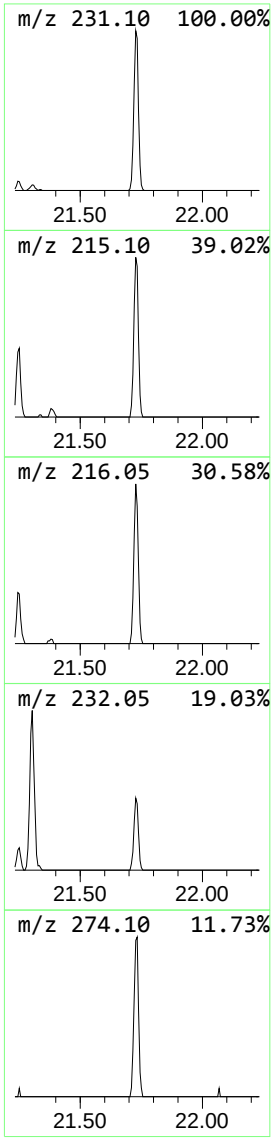
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Phenanthridine 6-chloro-2-m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.730	2.32 ng/ul	117214	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthridine 6-chloro-2-methyl...	231	C14H14ClN	035417-77-7	50
2	2-Benzothiazolamine, N-(1-methyl...	231	C12H13N3S	084859-07-4	46
3	2-[(Methylamino)methylene]thiazo...	231	C11H9N3OS	072740-41-1	46
4	2,4(1H,3H)-Pyridinedione, 1-(4-m...	231	C13H13NO3	1000318-74-6	43
5	Furane-2-carboxaldehyde, 5-(2-me...	231	C12H9NO4	329222-70-0	43





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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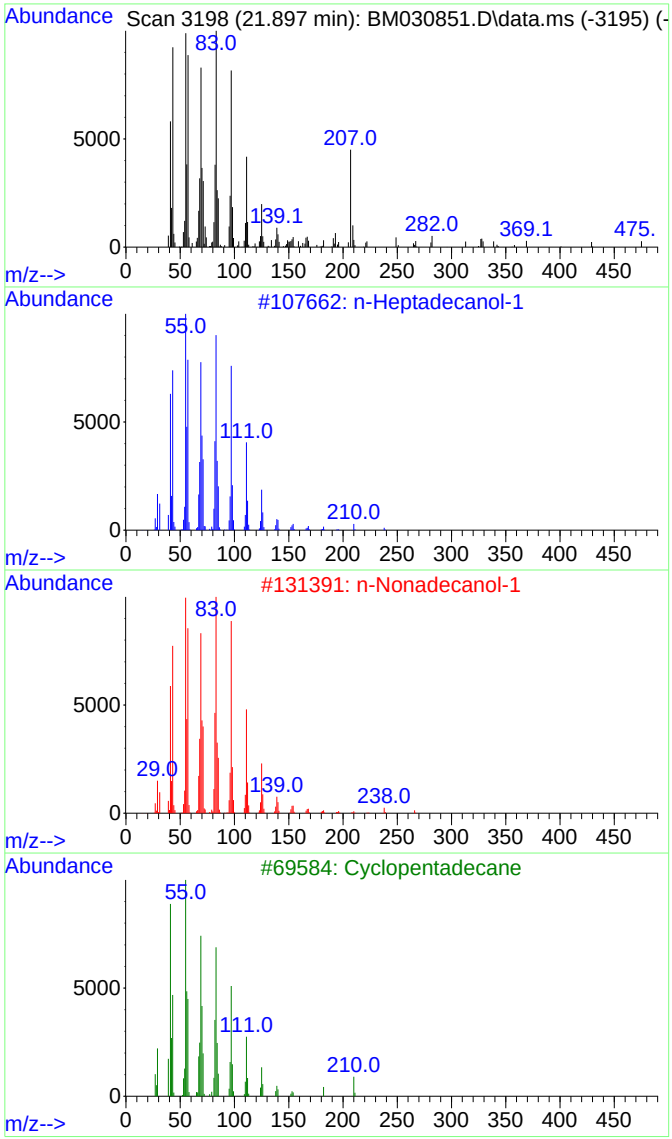
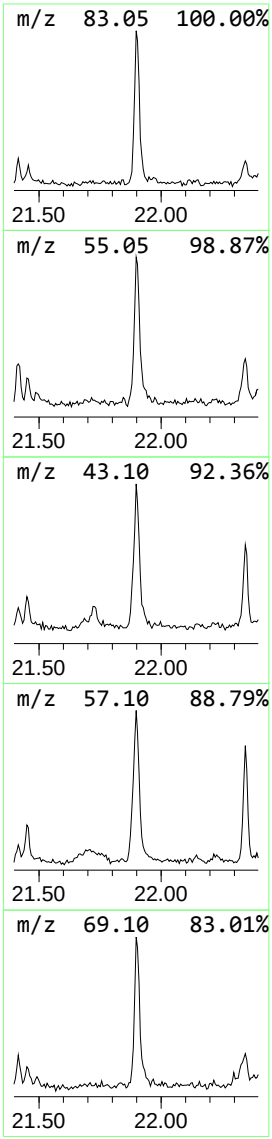
Peak Number 7 n-Heptadecanol-1 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.900	2.76 ng/ul	139246	Chrysene-d12	21.303

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Cyclopentadecane	210	C15H30	000295-48-7	92
4	1-Heneicosanol	312	C21H44O	015594-90-8	90
5	1-Hexadecanol	242	C16H34O	036653-82-4	83





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Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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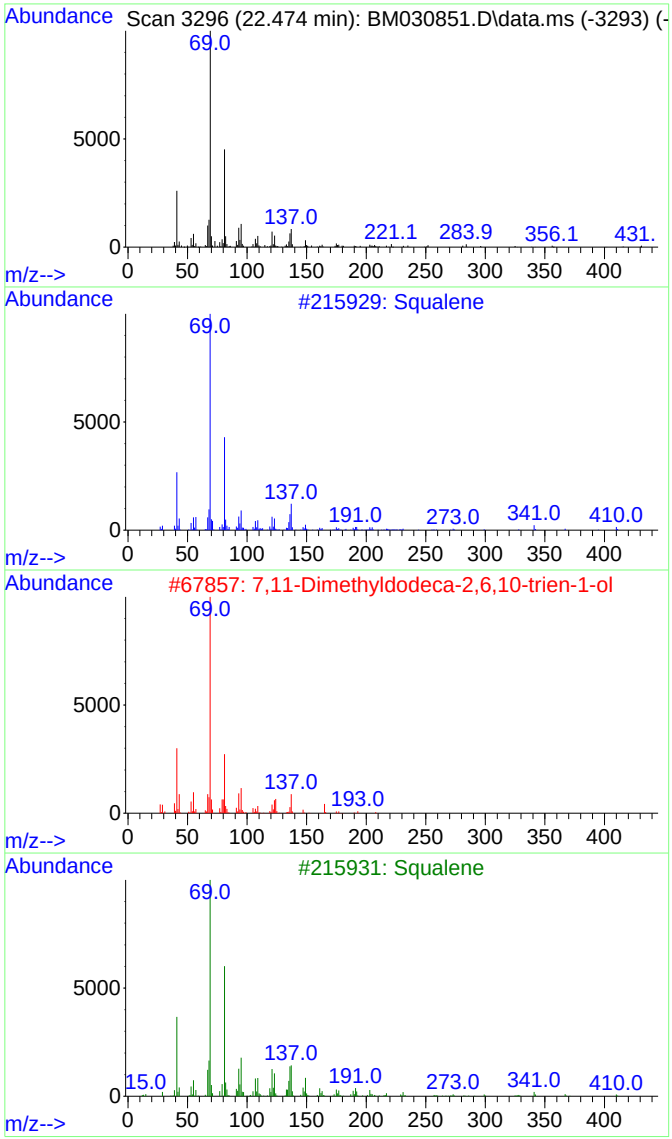
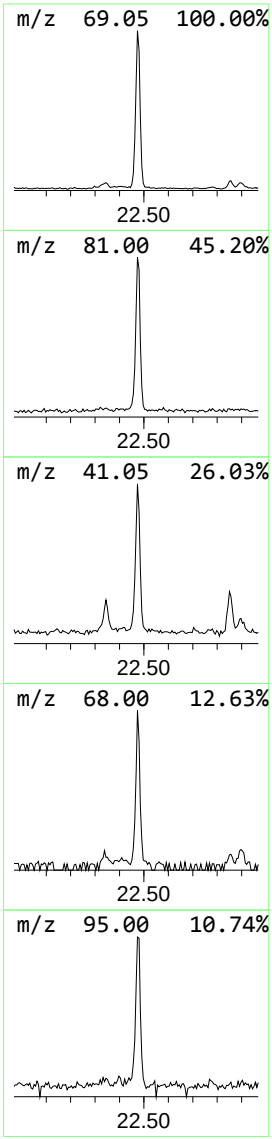
Peak Number 8 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.470	2.82 ng/ul	158551	Perylene-d12	23.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	90
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	87
3	Squalene	410	C30H50	000111-02-4	83
4	Squalene	410	C30H50	000111-02-4	83
5	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78





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Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGDS1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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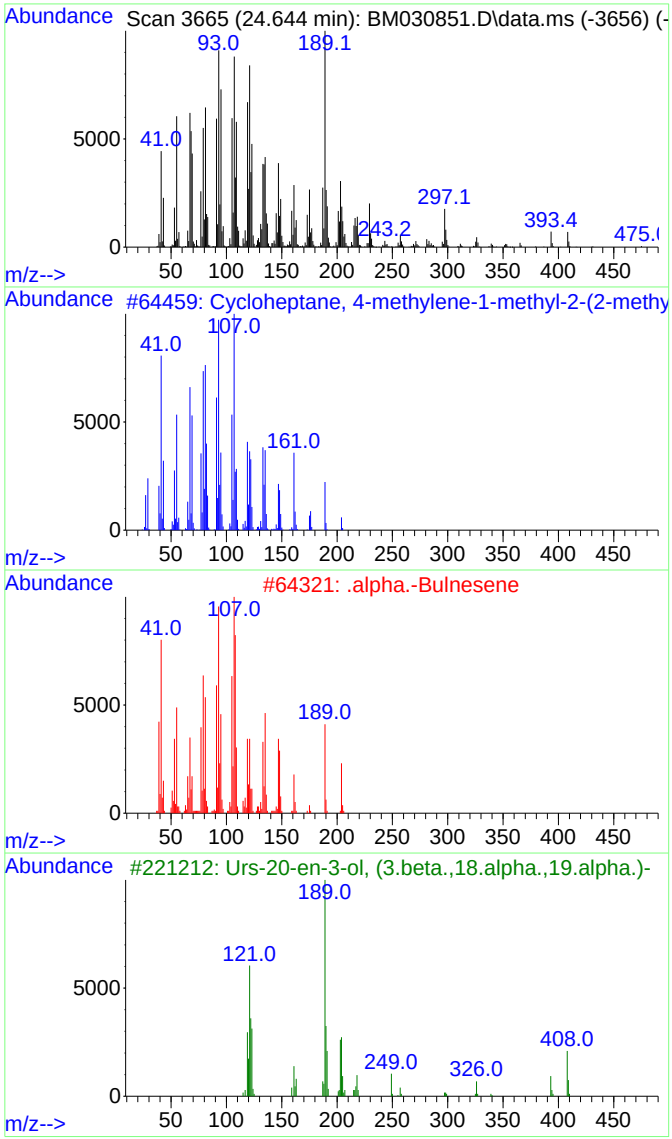
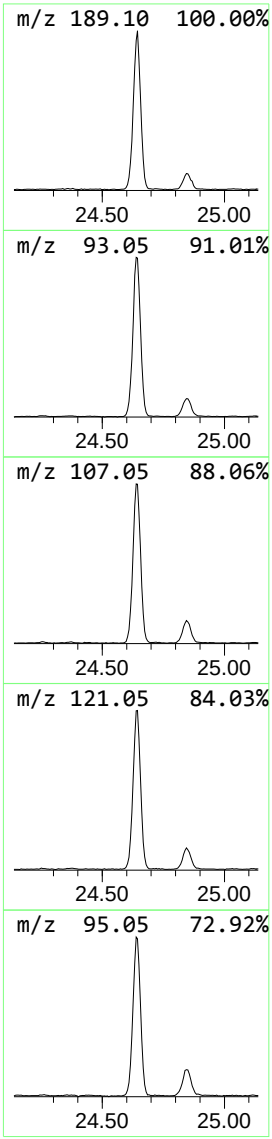
Peak Number 9 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.640	71.69 ng/ul	4030140	Perylene-d12	23.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptane, 4-methylene-1-meth...	204	C15H24	1000159-38-5	49
2	.alpha.-Bulnesene	204	C15H24	1000374-19-9	45
3	Urs-20-en-3-ol, (3.beta.,18.alph...	426	C30H50O	000464-98-2	43
4	Guaia-1(10),11-diene	204	C15H24	1000374-19-7	43
5	1,5-Cycloundecadiene, 9-(1-methy...	190	C14H22	062338-55-0	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM070621\
Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGDS1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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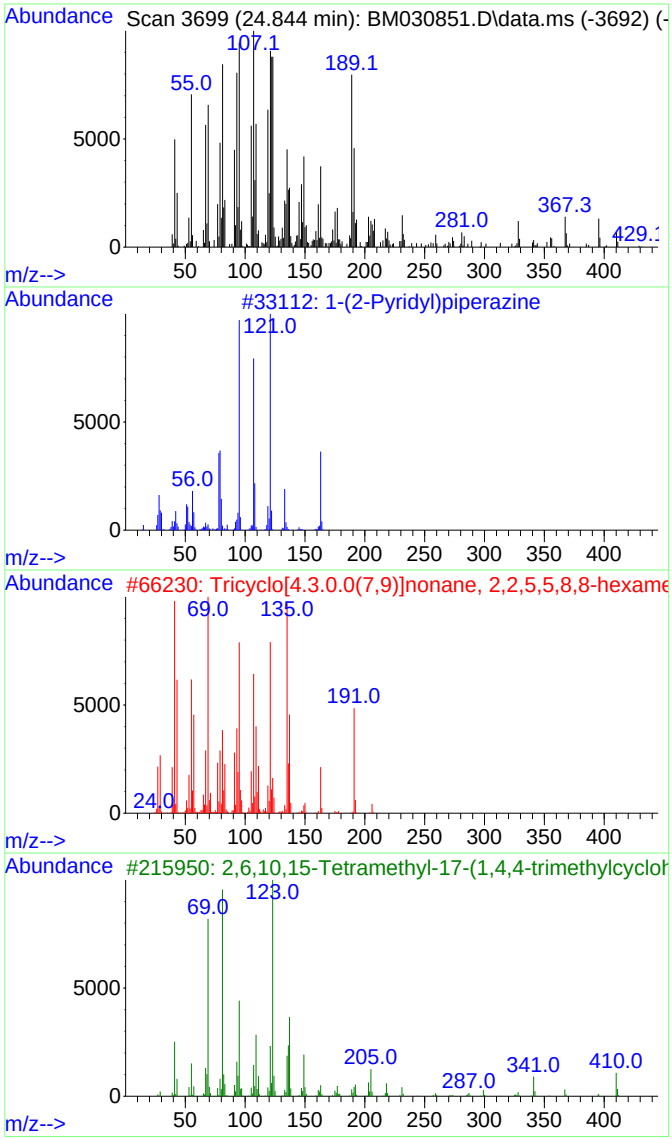
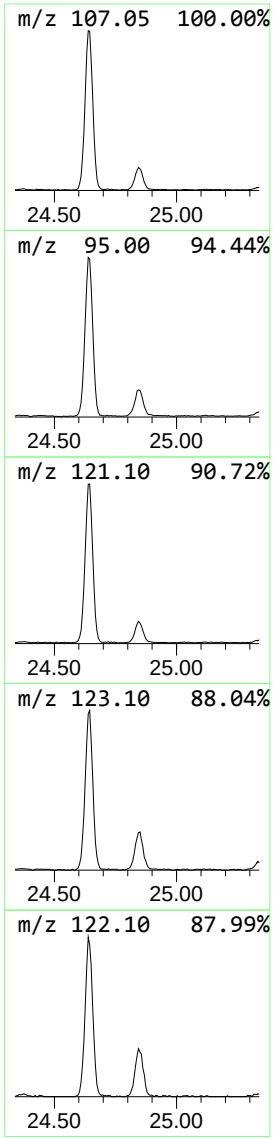
Peak Number 10 unknown-03 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.840	13.14 ng/ul	738631	Perylene-d12	23.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	42
2	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	42
3	2,6,10,15-Tetramethyl-17-(1,4,4-...	410	C30H50	1000195-23-2	25
4	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	22
5	Cyclohexane, 1,2-dimethyl-3,5-bi...	192	C14H24	074806-55-6	18





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Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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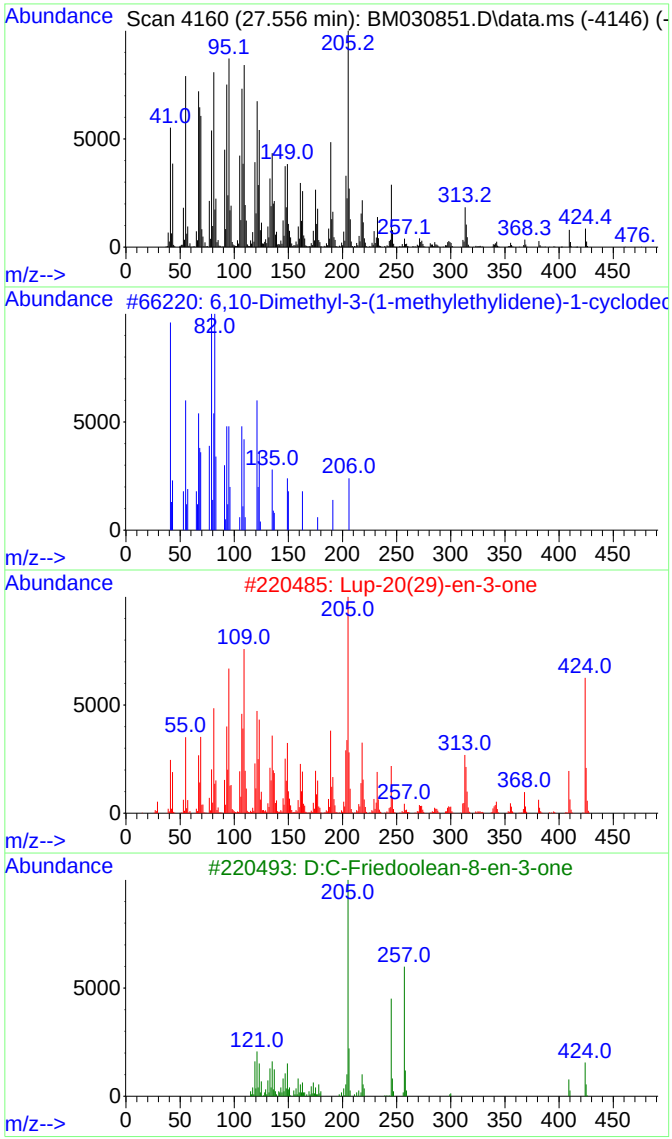
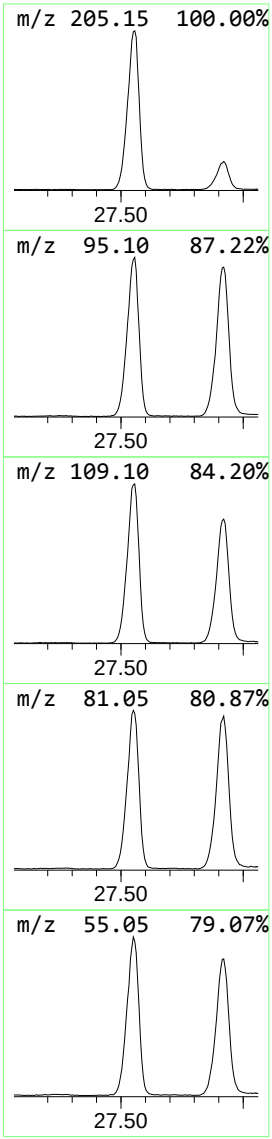
Peak Number 11 6,10-Dimethyl-3-(1-methylet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.560	202.59 ng/ul	11388800	Perylene-d12	23.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	87
2	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	86
3	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	74
4	Guaia-9,11-diene	204	C15H24	1000374-19-8	60
5	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	45





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Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
BGDS1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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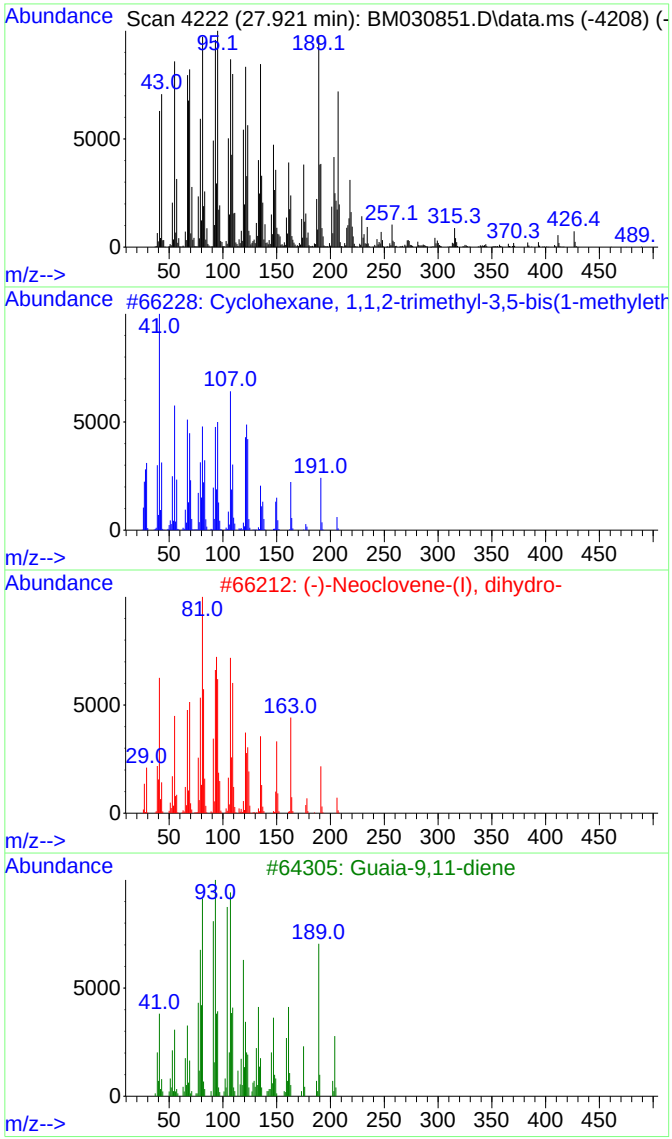
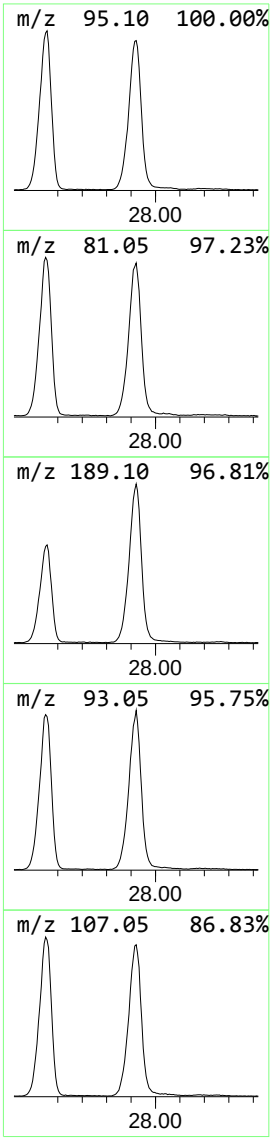
Peak Number 12 Cyclohexane, 1,1,2-trimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.920	209.12 ng/ul	11755900	Perylene-d12	23.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,2-trimethyl-3,5...	206	C15H26	062337-97-7	70
2	(-)-Neoclovene-(I), dihydro-	206	C15H26	1000152-82-1	64
3	Guaia-9,11-diene	204	C15H24	1000374-19-8	53
4	(-)-Neoclovene-(II), dihydro-	206	C15H26	1000152-83-6	47
5	Longifolenaldehyde	220	C15H24O	019890-84-7	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM070621\
Data File : BM030851.D
Acq On : 07 Jul 2021 10:56
Operator : CG/JU
Sample : M2854-01
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : BGDS1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SFAM-EPA-BM070621.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.020	3.7	ng/ul	168870	4	17.133	921363	20.0
Hexanedioic aci...	20.520	5.7	ng/ul	286300	5	21.303	1010340	20.0
(DEL) Alkane: S...	21.010	5.7	ng/ul	288544	5	21.303	1010340	20.0
Naphthalene, 1,...	21.160	7.0	ng/ul	354619	5	21.303	1010340	20.0
unknown-01	21.240	14.8	ng/ul	749307	5	21.303	1010340	20.0
Phenanthridine ...	21.730	2.3	ng/ul	117214	5	21.303	1010340	20.0
n-Heptadecanol-1	21.900	2.8	ng/ul	139246	5	21.303	1010340	20.0
Squalene	22.470	2.8	ng/ul	158551	6	23.550	1124310	20.0
unknown-02	24.640	71.7	ng/ul	4030140	6	23.550	1124310	20.0
unknown-03	24.840	13.1	ng/ul	738631	6	23.550	1124310	20.0
6,10-Dimethyl-3...	27.560	202.6	ng/ul	11388800	6	23.550	1124310	20.0
Cyclohexane, 1,...	27.920	209.1	ng/ul	11755900	6	23.550	1124310	20.0