LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

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\SOM-EPA-BM112719MA.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.034	22	25	34	rVB	72376	101663	0.21%	0.052%
2	3.652	125	130	138	rVB	53563	96128	0.20%	0.050%
3	4.646	295	299	303	rBV	52579	76201	0.16%	0.039%
4	6.675	637	644	660	rBV	1069761	1855889	3.88%	0.957%
5	6.834	665	671	689	rVV	924641	1516780	3.17%	0.782%
6	7.022	696	703	718	rBV	1219247	1969910	4.12%	1.016%
7	7.487	775	782	793	rBV	1182359	1881840	3.93%	0.970%
8	8.204	896	904	918	rBV	985115	1660482	3.47%	0.856%
9	8.322	918	924	933	rVB2	43514	86530	0.18%	0.045%
10	8.640	971	978	989	rBV	1058773	1807353	3.78%	0.932%
11	9.357	1092	1100	1118	rBV	870062	1525107	3.19%	0.786%
12	9.892	1183	1191	1210	rBV	1376362	2437519	5.10%	1.257%
13	10.257	1246	1253	1266	rVB	1609925	2658626	5.56%	1.371%
14	10.410	1270	1279	1306	rBV	930855	1916377	4.01%	0.988%
15	13.569	1810	1816	1820	rBV	2638397	3609346	7.55%	1.861%
16	13.616	1820	1824	1837	rVB	994403	1393186	2.91%	0.718%
17	13.833	1854	1861	1873	rBV	3020705	4523393	9.46%	2.332%
18	14.145	1908	1914	1927	rBV	2405402	3543076	7.41%	1.827%
19	14.380	1948	1954	1976	rBV	670915	1424943	2.98%	0.735%
20	14.598	1986	1991	2004	rVB3	88381	177875	0.37%	0.092%
21	15.145	2078	2084	2098	rBV	3983928	5810332	12.15%	2.996%
22	15.286	2100	2108	2121	rVV	915603	1368935	2.86%	0.706%
23	15.392	2121	2126	2132	rVB	42265	65774	0.14%	0.034%
24	16.898	2376	2382	2392	rBV	2889278	4105826	8.59%	2.117%
25	16.998	2393	2399	2415	rVV	4341166	6172375	12.91%	3.183%
26	17.827	2534	2540	2548	rBV	445708	743753	1.56%	0.384%
27	18.257	2609	2613	2616	rBV3	51997	56117	0.12%	0.029%
28	18.298	2616	2620	2626	rVB4	32878	55223	0.12%	0.028%
29	18.939	2726	2729	2733	rBV	51460	70314	0.15%	0.036%
30	19.033	2742	2745	2750	rVB	60159	73482	0.15%	0.038%
31	19.121	2755	2760	2768	rBV2	114098	202339	0.42%	0.104%
32	19.192	2768	2772	2776	rVB	53384	70139	0.15%	0.036%
33	19.304	2785	2791	2804	rBV2	5735907	7847422	16.41%	4.046%
34	20.433	2978	2983	2988	rVB	486019	675449	1.41%	0.348%

LSC Area Percent Report

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Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

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\SOM-EPA-BM112719MA.M
Title : SVOA CALIBRATION

35	20.715	3028	3031	3034	rBV4	110134	144386	0.30%	0.074%
36	20.756	3034	3038	3047	rVV	1221496	1894057	3.96%	0.977%
37	20.851	3049	3054	3061	rBV	940146	1286361	2.69%	0.663%
38	20.974	3072	3075	3079	rVB3	156944	201403	0.42%	0.104%
39	21.045	3085	3087	3090	rBV	88662	99443	0.21%	0.051%
40	21.109	3093	3098	3106	rVV	3589617	4725416	9.88%	2.437%
41	21.292	3126	3129	3132	rBV2	127372	154350	0.32%	0.080%
42	21.709	3197	3200	3207	rBV	478067	595016	1.24%	0.307%
43	21.850	3221	3224	3230	rBV5	222442	278907	0.58%	0.144%
44	22.150	3273	3275	3280	rVB	239319	282418	0.59%	0.146%
45	22.274	3291	3296	3302	rVB	1690841	2109935	4.41%	1.088%
46	22.633	3354	3357	3362	rVB	388692	523271	1.09%	0.270%
47	23.121	3433	3440	3446	rBV	4685777	8471081	17.71%	4.368%
48	23.250	3456	3462	3470	rVB	2990868	5365312	11.22%	2.767%
49	23.539	3507	3511	3519	rVB4	471391	804012	1.68%	0.415%
50	26.503	4002	4015	4023	rBV2	15619853	47823777	100.00%	24.660%
51	26.585	4023	4029	4039	rVB	5548733	14537614	30.40%	7.496%
52	26.850	4063	4074	4085	rBV5	3563611	14517232	30.36%	7.486%
53	26.980	4088	4096	4120	rVB4	5219472	18901926	39.52%	9.746%
54	28.844	4405	4413	4436	rVB2	2219747	9640615	20.16%	4.971%

Sum of corrected areas: 193936236

LSC Report - Integrated Chromatogram

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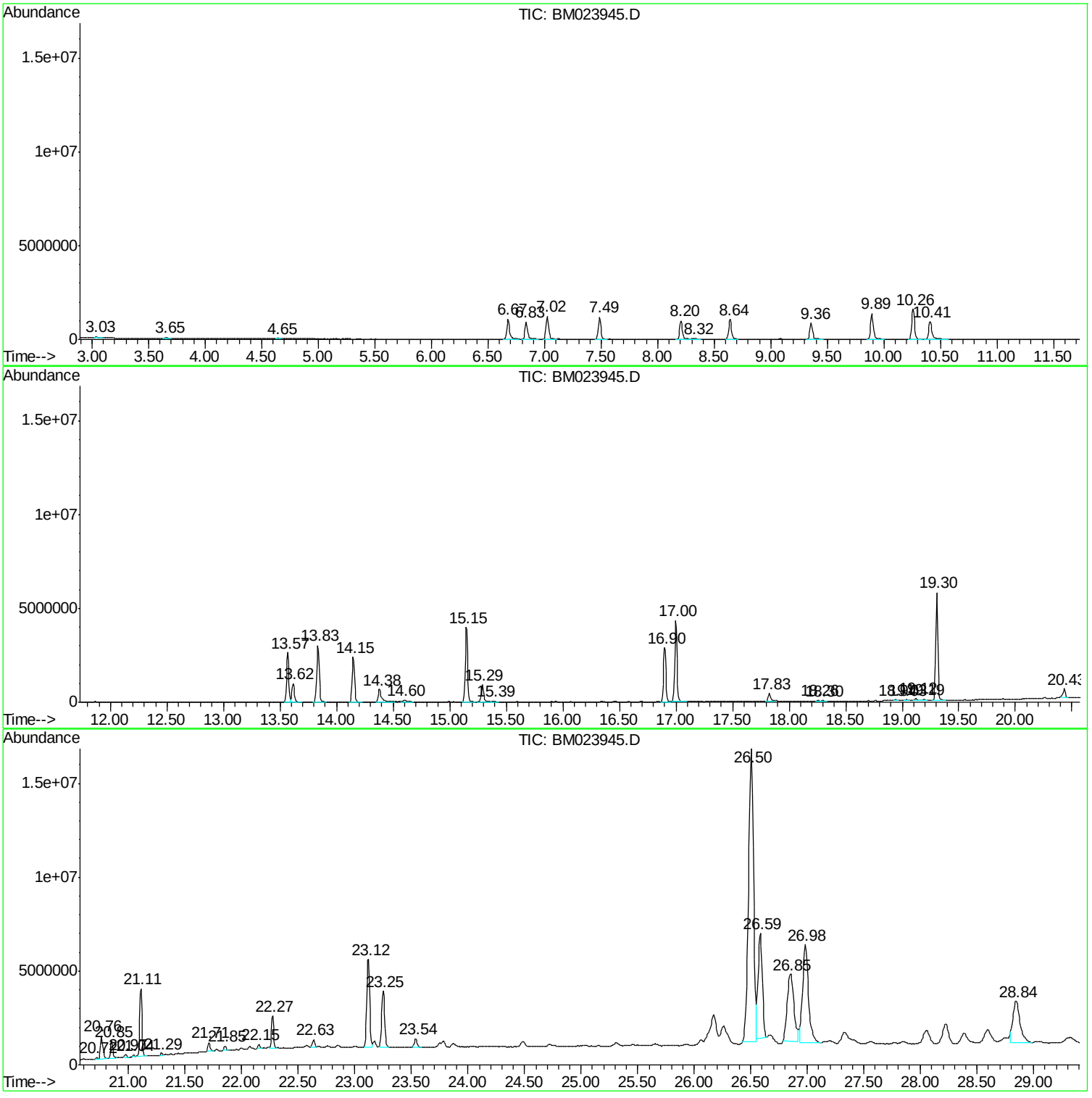
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

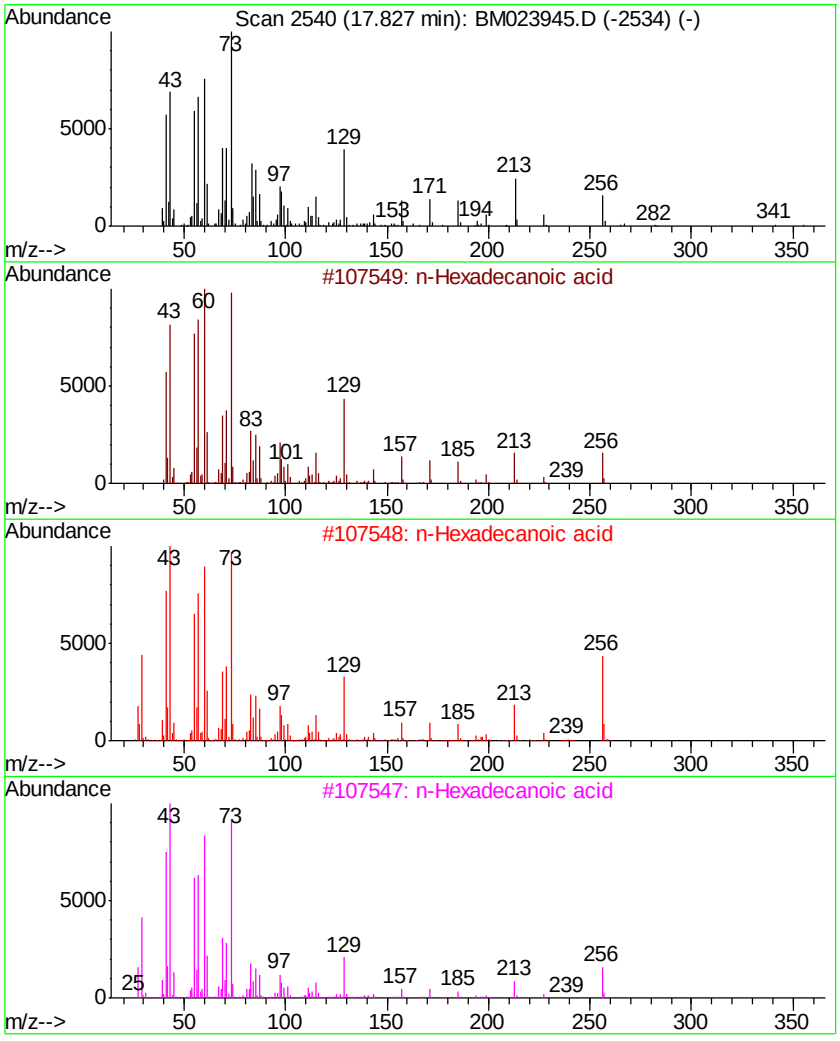
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

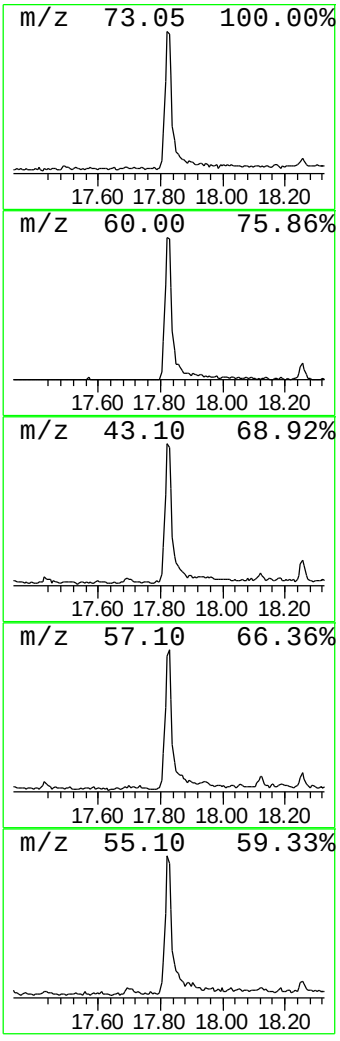
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	3.62 ng/ul	743753	Phenanthrene-d10	16.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

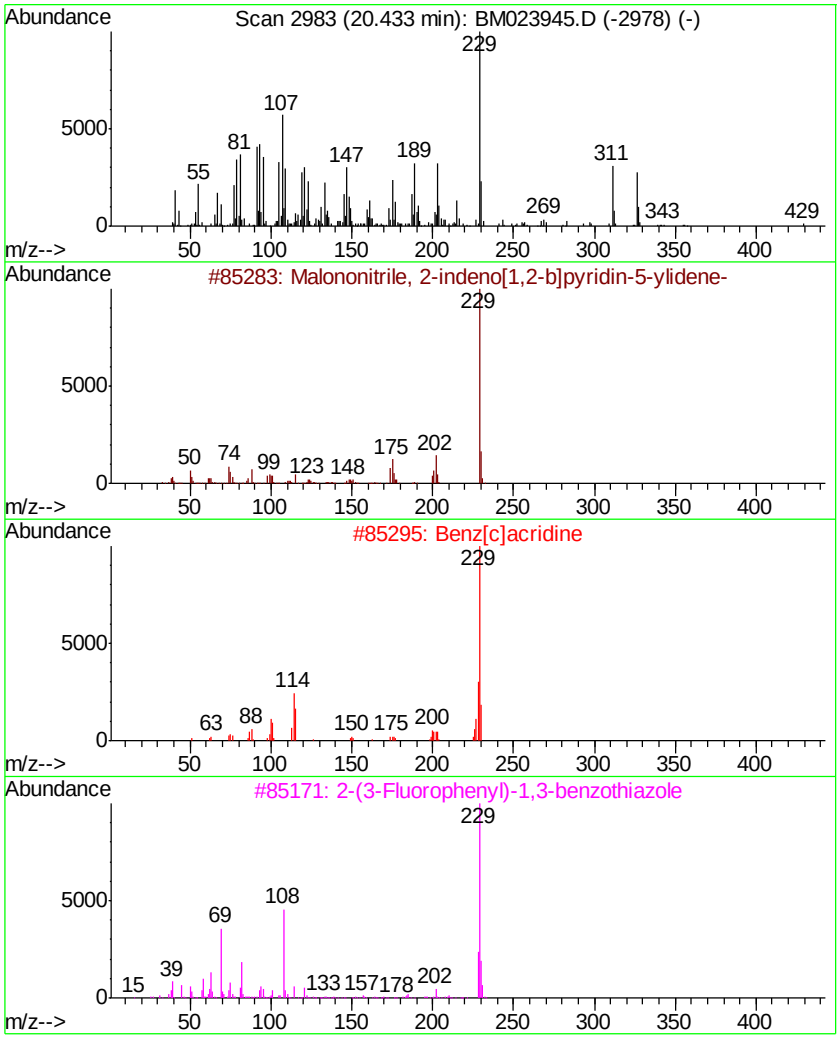
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

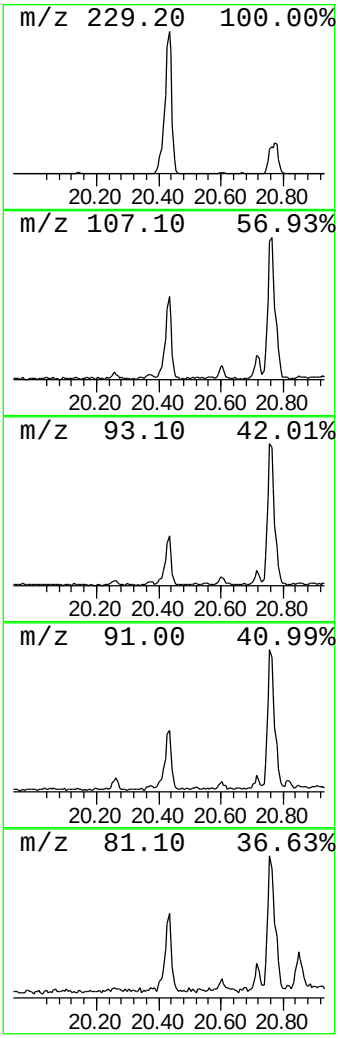
****

Peak Number 2 unknown-01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	2.86 ng/ul	675449	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Malononitrile, 2-indeno[1,2-b]py...	229	C15H7N3	1000316-60-9	27
2	Benz[c]acridine	229	C17H11N	000225-51-4	22
3	2-(3-Fluorophenyl)-1,3-benzothia...	229	C13H8FNS	1000298-18-6	22
4	Indan, 6-tert-butyl-1,1,3,4-tetr...	300	C22H36	029577-23-9	22
5	Benzo(a)acridine	229	C17H11N	000225-11-6	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

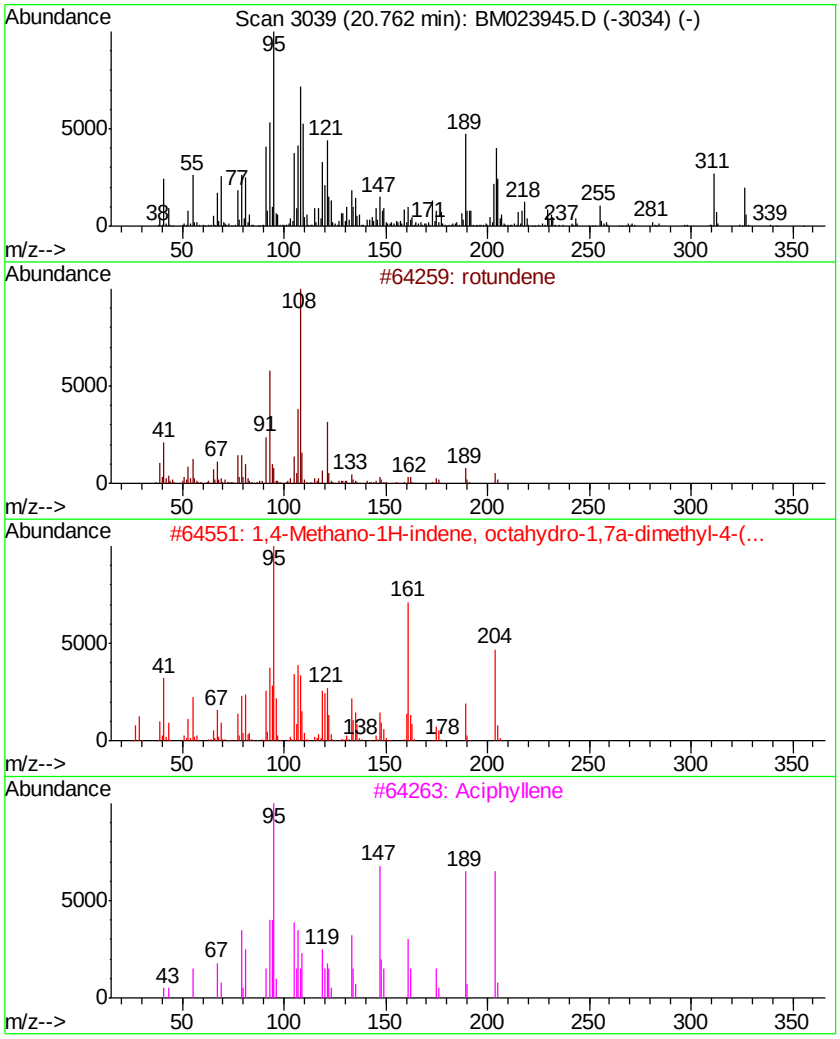
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

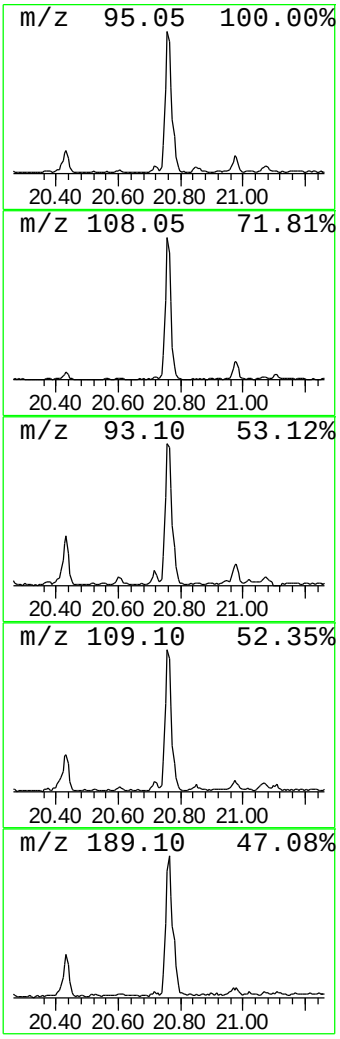
****

Peak Number 3 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	8.02 ng/ul	1894060	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	rotundene	204	C15H24	1000374-17-0	46
2	1,4-Methano-1H-indene, octahydro...	204	C15H24	087064-18-4	42
3	Aciphyllene	204	C15H24	087745-31-1	42
4	2,10-Bornanediol, exo-	170	C10H18O2	001925-39-9	38
5	1H-Benzocycloheptene, 2,4a,5,6,7...	204	C15H24	003853-83-6	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

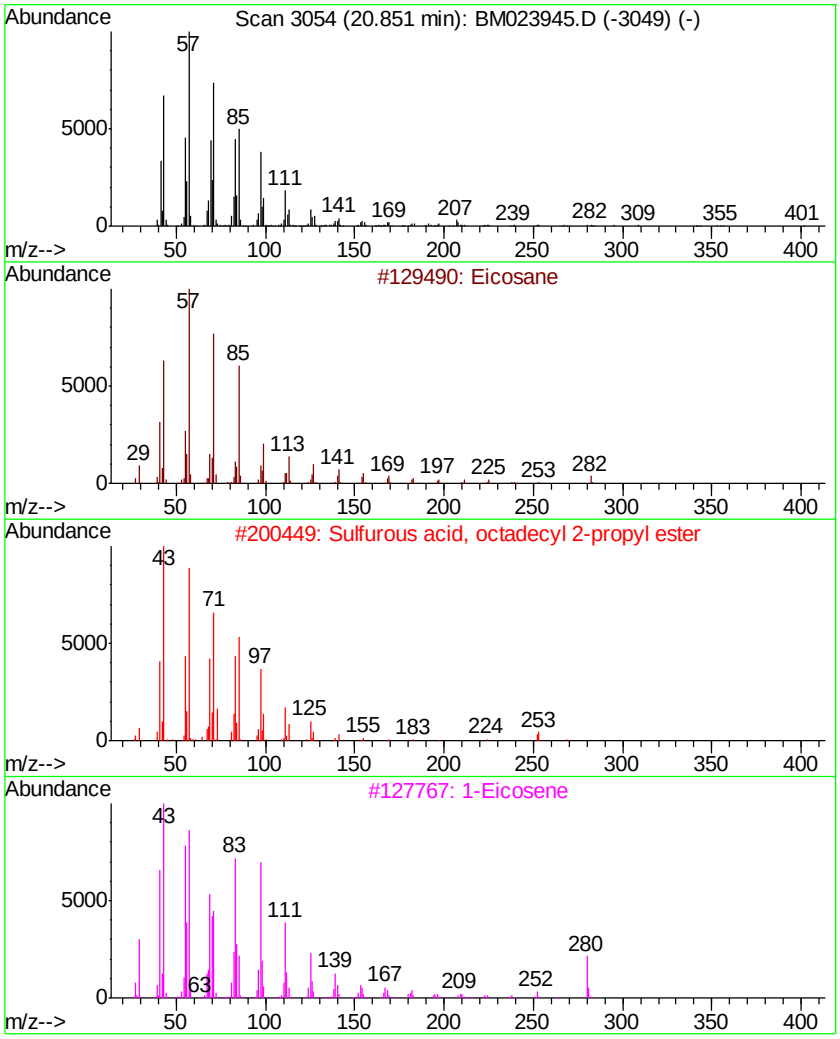
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

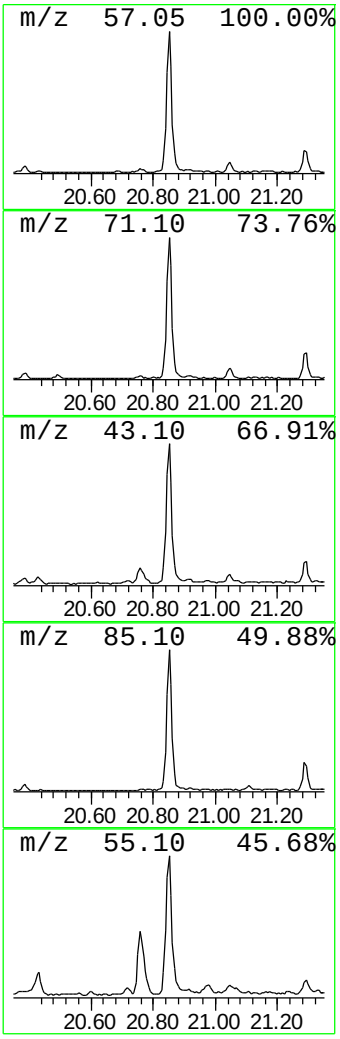
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	5.44 ng/ul	1286360	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	92
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	91
3	1-Eicosene	280	C20H40	003452-07-1	89
4	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	87
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87





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Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

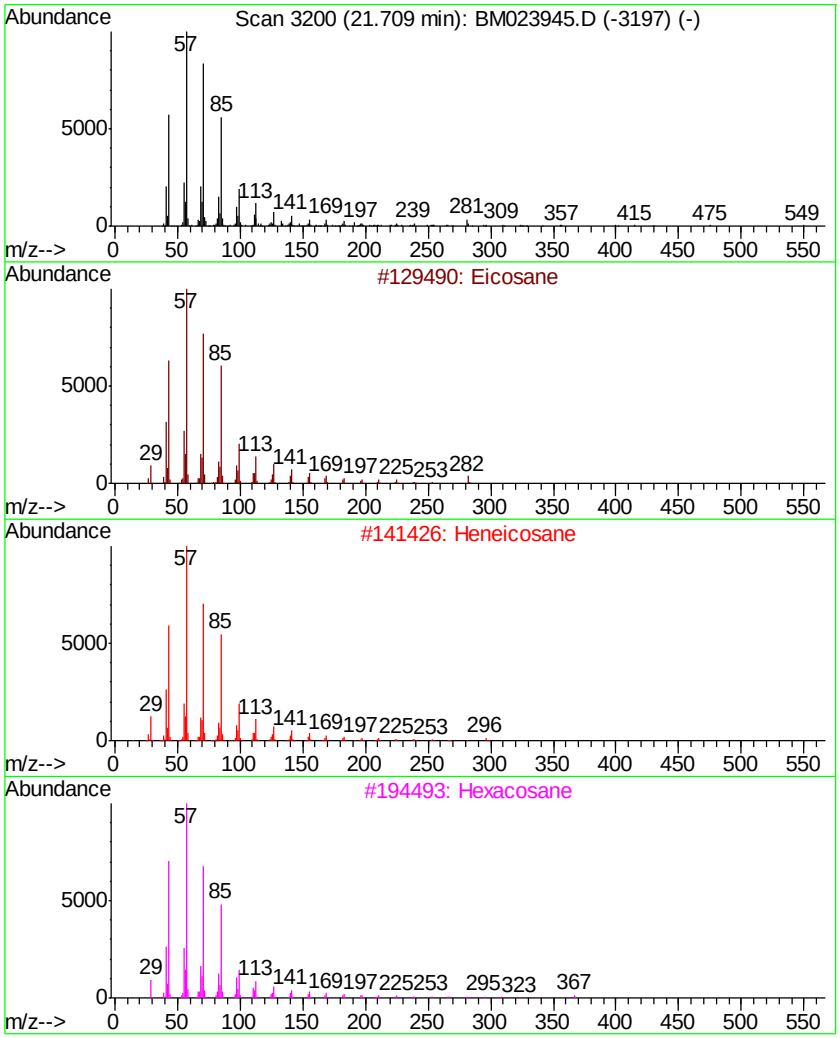
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

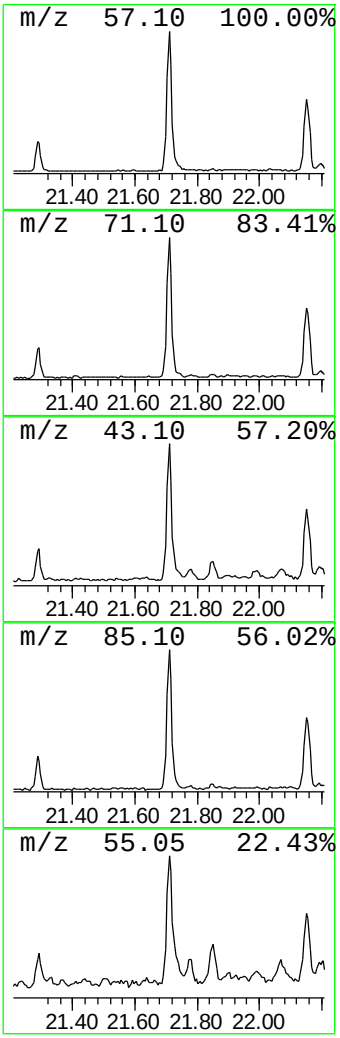
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	2.52 ng/ul	595016	Chrysene-d12	21.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Hexadecane	226	C16H34	000544-76-3	91
5	Octadecane	254	C18H38	000593-45-3	91





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Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

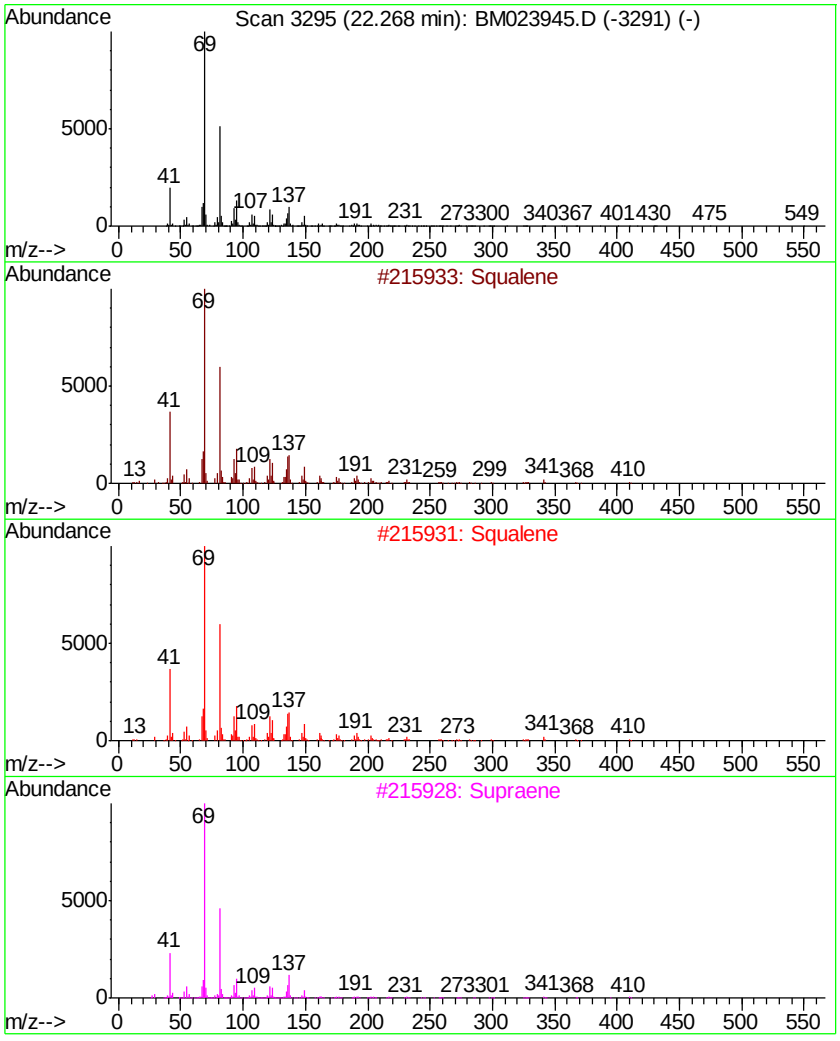
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

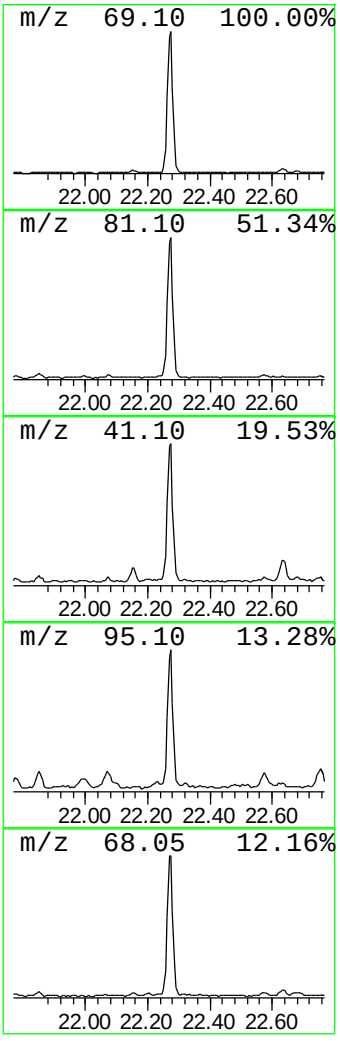
****

Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.27	7.87 ng/ul	2109940	Perylene-d12	23.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Squalene	410	C30H50	000111-02-4	95
3	Supraene	410	C30H50	007683-64-9	91
4	Squalene	410	C30H50	000111-02-4	91
5	Squalene	410	C30H50	000111-02-4	91





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ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

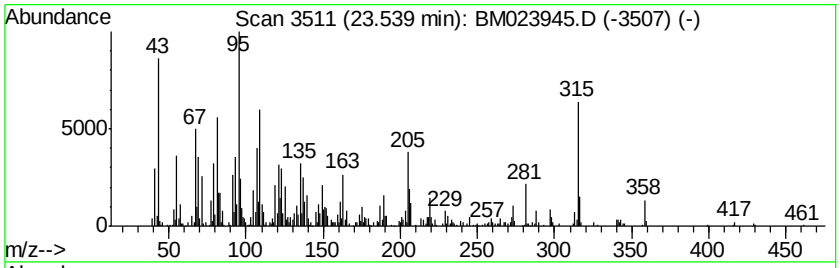
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

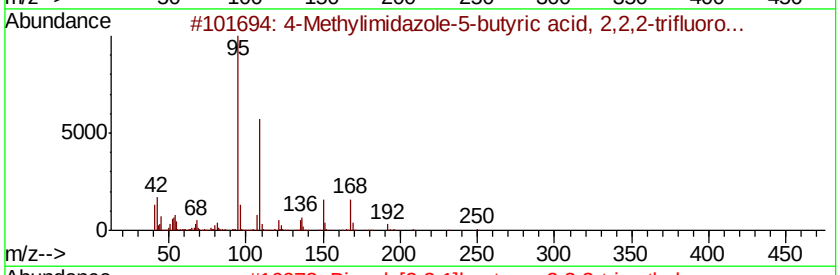
****

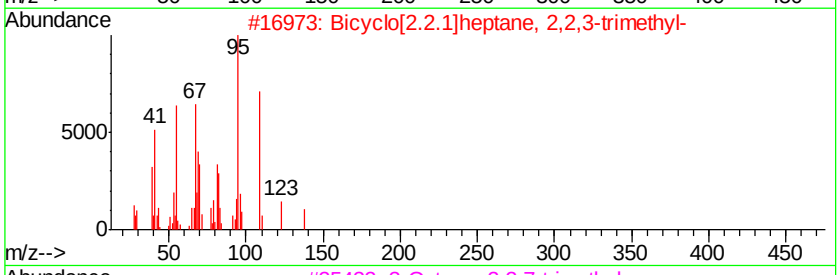
Peak Number 7 unknown-03 Concentration Rank 10

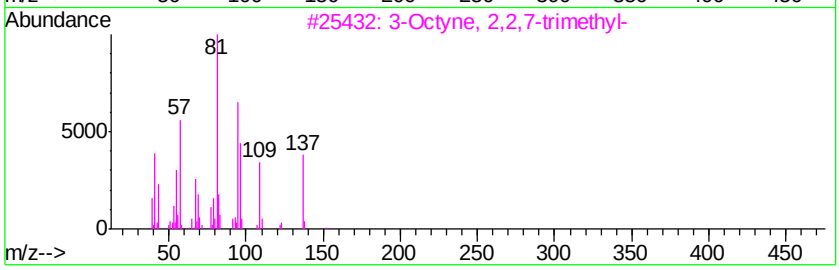
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.54	3.00 ng/ul	804012	Perylene-d12	23.25

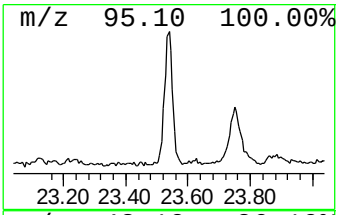
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Methylimidazole-5-butyric acid...	250	C10H13F3N2O2	1000129-15-9	35
2	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	000473-19-8	30
3	3-Octyne, 2,2,7-trimethyl-	152	C11H20	055402-13-6	27
4	cis-Z-.alpha.-Bisabolene epoxide	220	C15H24O	1000131-71-2	22
5	Ledol	222	C15H26O	000577-27-5	22

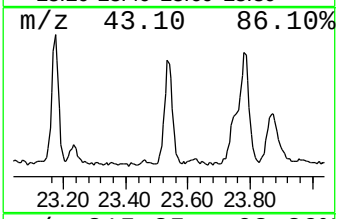


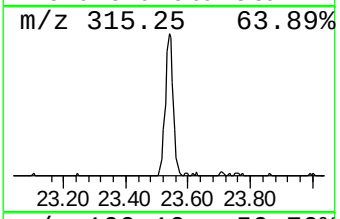


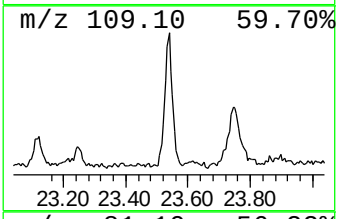


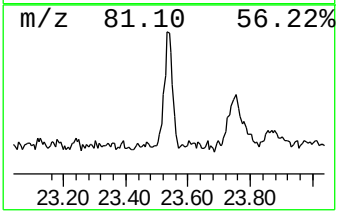












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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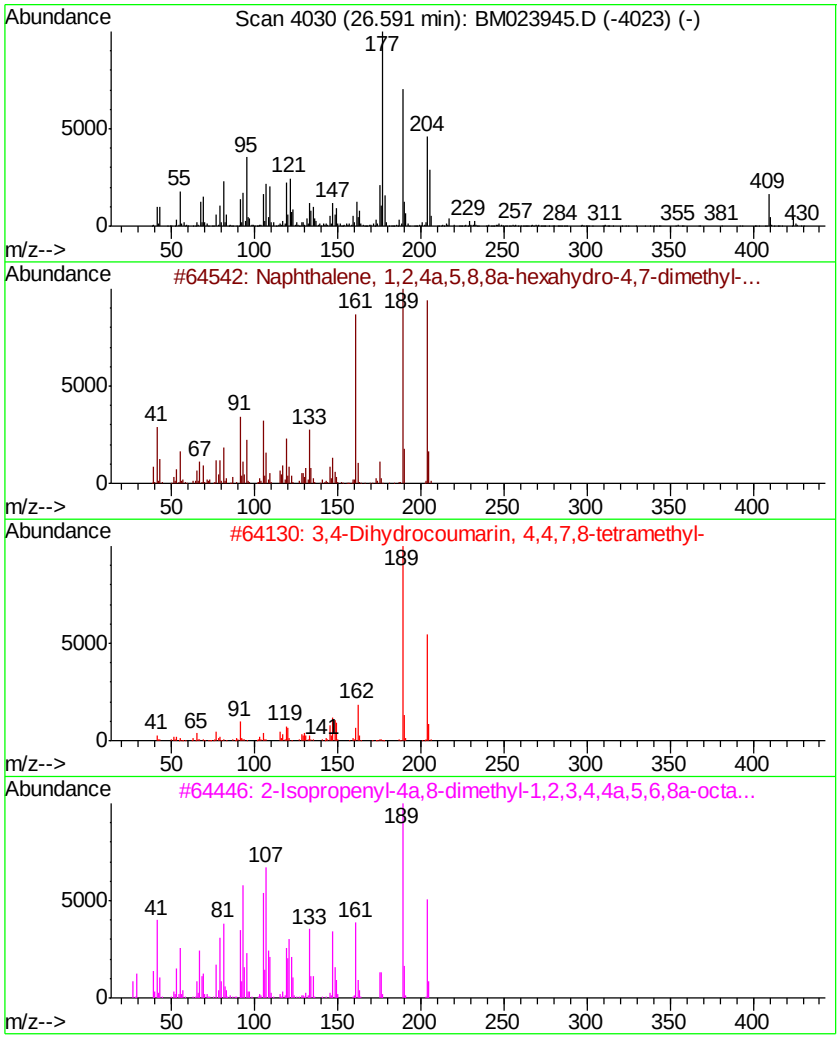
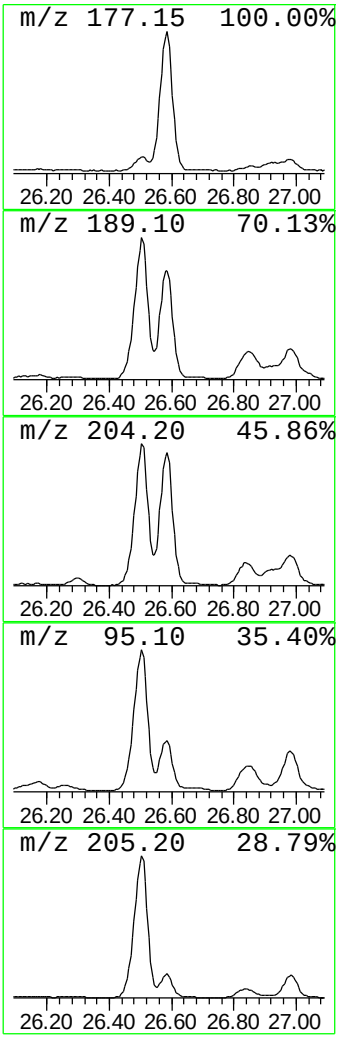
Peak Number 9 unknown-04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.59	54.19 ng/ul	14537600	Perylene-d12	23.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	005951-61-1	30
2	3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	30
3	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	30
4	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	27
5	2,10,10-Trimethyltricyclo[7.1.1....	204	C14H20O	1000210-81-9	22





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Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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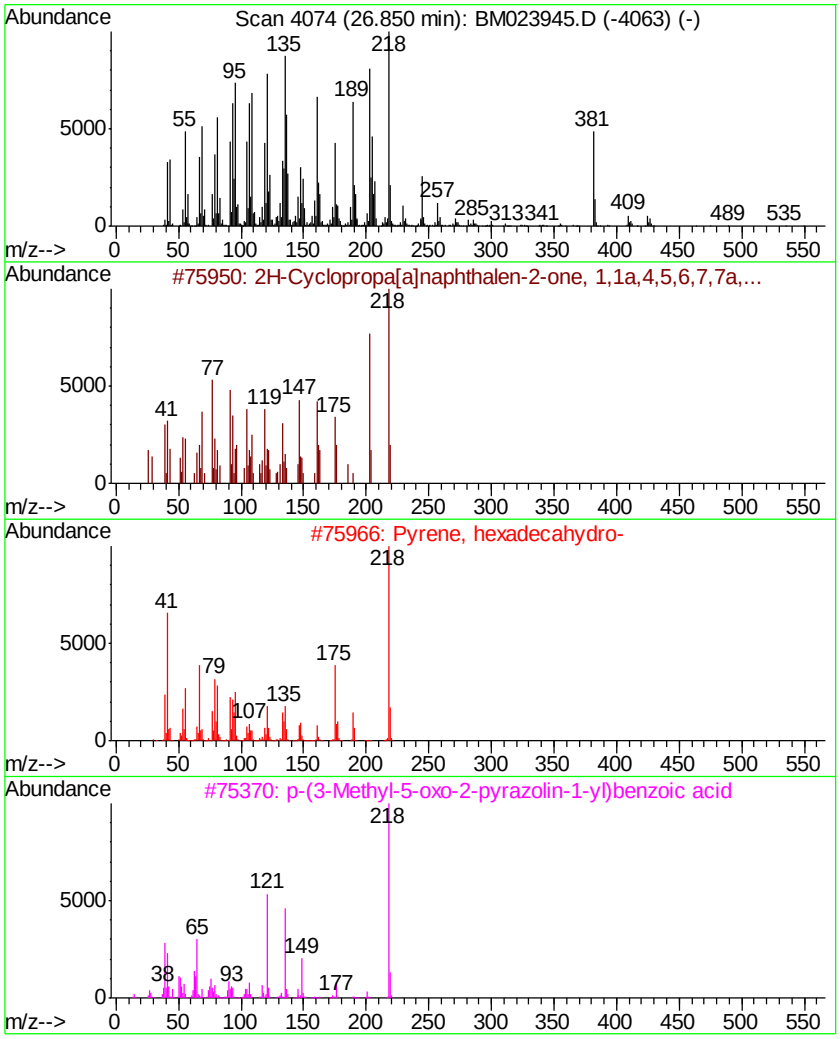
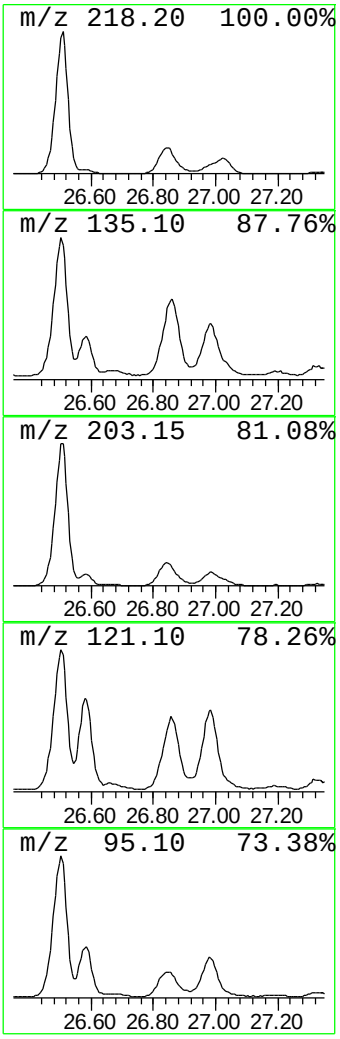
Peak Number 10 unknown-05 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.85	54.12 ng/ul	14517200	Perylene-d12	23.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	38
2	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	35
3	p-(3-Methyl-5-oxo-2-pyrazolin-1-...	218	C11H10N2O3	060875-16-3	25
4	[1,2,4]Triazolo[4,3-b][1,2,4]tri...	203	C8H5N5S	1000338-28-4	20
5	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	18





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Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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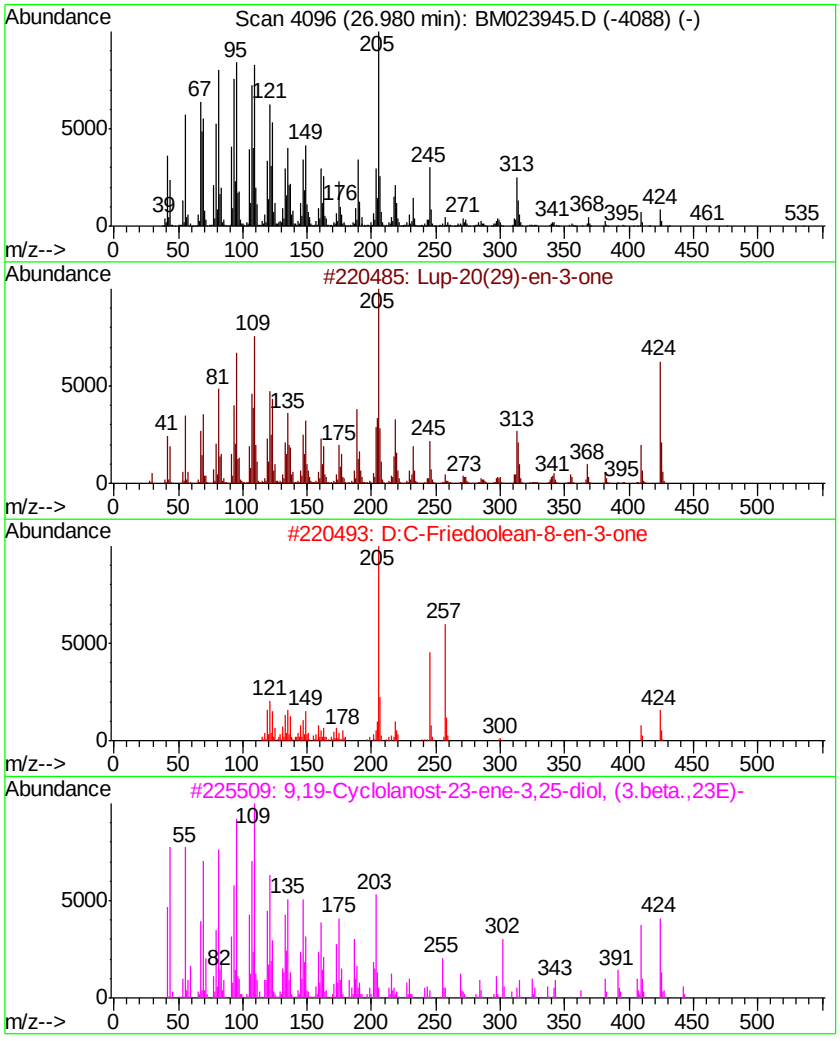
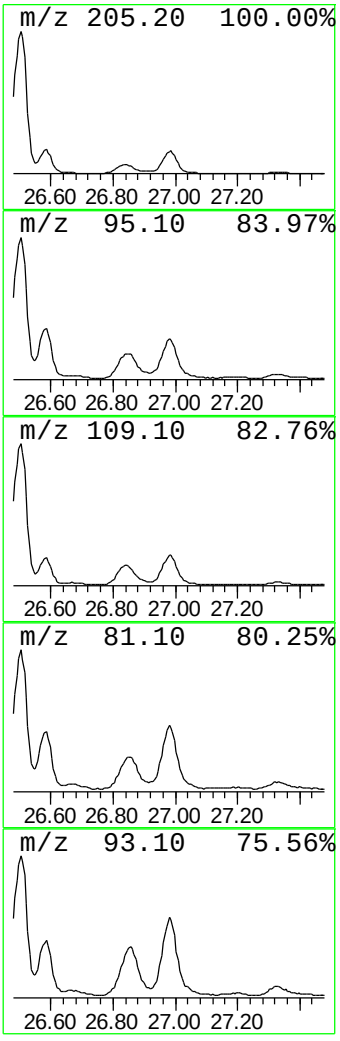
Peak Number 11 Lup-20(29)-en-3-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.98	70.46 ng/ul	18901900	Perylene-d12	23.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	95
2	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	68
3	9,19-Cyclolanost-23-ene-3,25-dio...	442	C30H50O2	054482-57-4	50
4	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	49
5	Dimethyl{bis[(4,8,8-trimethyldec...	500	C32H56O2Si	1000364-69-0	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.M
Quant Title : SVOA CALIBRATION

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

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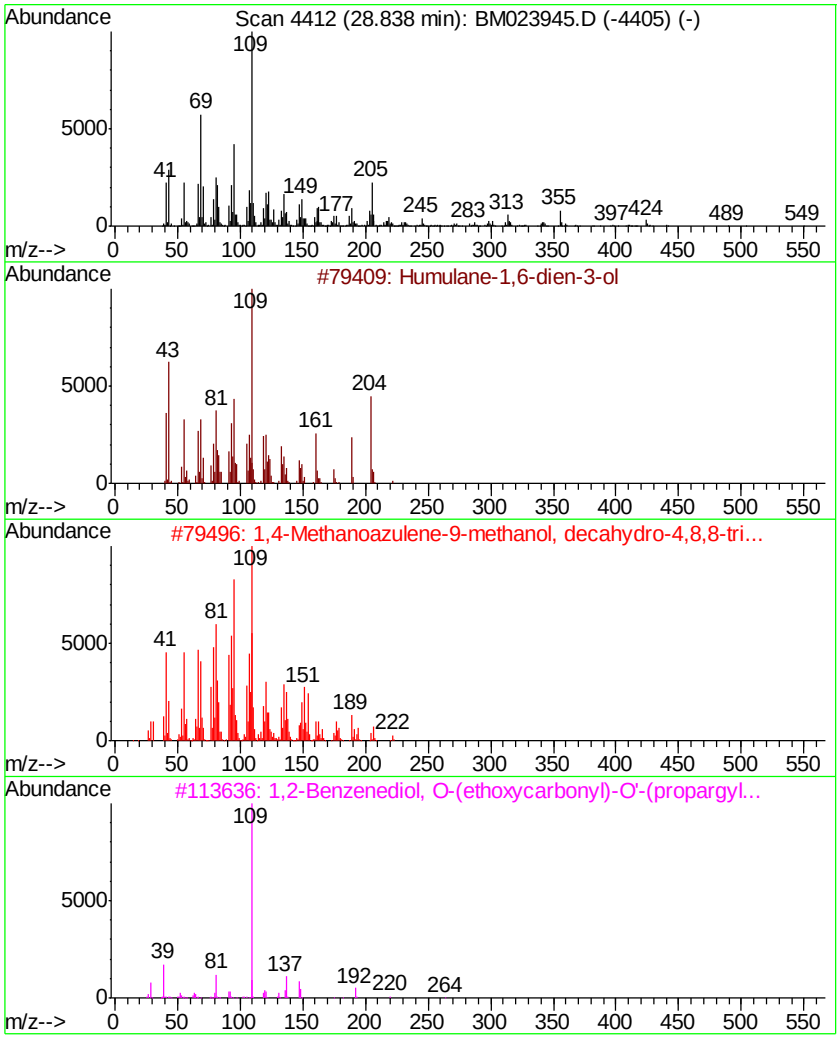
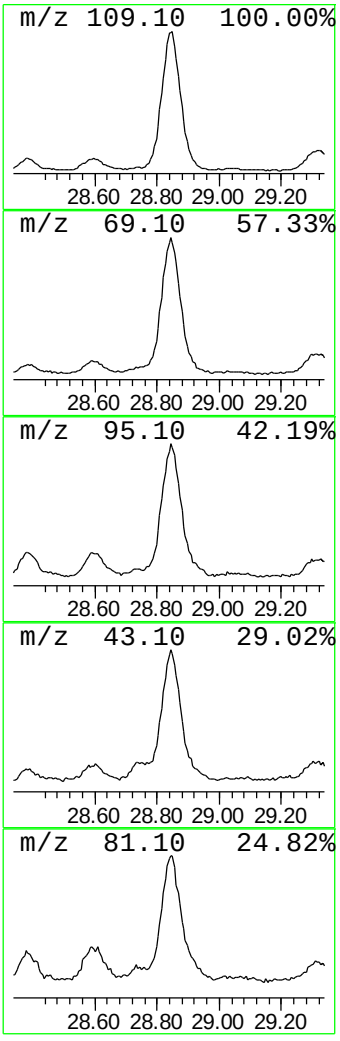
Peak Number 12 Humulane-1,6-dien-3-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.84	35.94 ng/ul	9640620	Perylene-d12	23.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Humulane-1,6-dien-3-ol	222	C15H26O	1000140-23-1	59
2	1,4-Methanoazulene-9-methanol, d...	222	C15H26O	001139-17-9	43
3	1,2-Benzenediol, O-(ethoxycarbon...	264	C13H12O6	1000329-71-6	42
4	(+)-(Z)-Longipinane	206	C15H26	1000156-12-3	38
5	Cyclohexanecarboxylic acid, 4-(c...	204	C10H17ClO2	055590-77-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM112719\
Data File : BM023945.D
Acq On : 28 Nov 2019 10:42
Operator : JU
Sample : K5915-06
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : JLNW1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM112719MA.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 acid	17.83	3.6	ng/ul	743753	4	16.90	4105830	20.0
unknown-01	20.43	2.9	ng/ul	675449	5	21.11	4725420	20.0
unknown-02	20.76	8.0	ng/ul	1894060	5	21.11	4725420	20.0
(DEL) Alkane: Str...	20.85	5.4	ng/ul	1286360	5	21.11	4725420	20.0
(DEL) Alkane: Str...	21.71	2.5	ng/ul	595016	5	21.11	4725420	20.0
Squalene	22.27	7.9	ng/ul	2109940	6	23.25	5365310	20.0
unknown-03	23.54	3.0	ng/ul	804012	6	23.25	5365310	20.0
unknown-04	26.59	54.2	ng/ul	14537600	6	23.25	5365310	20.0
unknown-05	26.85	54.1	ng/ul	14517200	6	23.25	5365310	20.0
Lup-20(29)-en-3-one	26.98	70.5	ng/ul	18901900	6	23.25	5365310	20.0
Humulane-1,6-dien...	28.84	35.9	ng/ul	9640620	6	23.25	5365310	20.0