LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM121518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.681	300	305	314	rBV	68676	95612	3.32%	0.306%
2	5.122	374	380	394	rBV	1808626	2572853	89.44%	8.229%
3	6.687	636	646	659	rBV	1663898	2781530	96.70%	8.896%
4	7.028	695	704	715	rBV	1773179	2828238	98.32%	9.045%
5	7.481	770	781	788	rBV	427829	682613	23.73%	2.183%
6	7.798	827	835	845	rBV	1347896	2154153	74.89%	6.889%
7	8.639	971	978	989	rBV	926716	1646158	57.23%	5.265%
8	10.251	1245	1252	1262	rBV	474272	827191	28.76%	2.646%
9	12.463	1621	1628	1634	rBV5	19065	37540	1.31%	0.120%
10	12.527	1634	1639	1651	rBV2	46619	101611	3.53%	0.325%
11	12.751	1670	1677	1687	rBV	1919436	2876508	100.00%	9.200%
12	13.163	1742	1747	1753	rBV4	15849	29740	1.03%	0.095%
13	13.227	1753	1758	1763	rVB4	17592	35196	1.22%	0.113%
14	13.616	1819	1824	1837	rVB	109486	176962	6.15%	0.566%
15	14.145	1906	1914	1922	rBV2	572376	932616	32.42%	2.983%
16	15.651	2164	2170	2182	rBV	1555664	2319692	80.64%	7.419%
17	15.986	2222	2227	2234	rBV2	38792	81003	2.82%	0.259%
18	16.327	2282	2285	2291	rBV6	18510	36490	1.27%	0.117%
19	16.821	2365	2369	2376	rBV5	33393	47925	1.67%	0.153%
20	16.909	2377	2384	2389	rVV2	678434	1039774	36.15%	3.325%
21	16.957	2389	2392	2396	rVV4	116601	158784	5.52%	0.508%
22	17.004	2397	2400	2404	rVB4	28719	43951	1.53%	0.141%
23	17.280	2442	2447	2454	rBV2	42171	62757	2.18%	0.201%
24	17.704	2510	2519	2525	rBV7	35460	77095	2.68%	0.247%
25	17.756	2525	2528	2533	rBV5	22521	33848	1.18%	0.108%
26	17.821	2534	2539	2551	rBV	370249	559147	19.44%	1.788%
27	18.121	2585	2590	2593	rBV7	17495	30190	1.05%	0.097%
28	18.774	2698	2701	2709	rVB4	53165	76321	2.65%	0.244%
29	18.845	2709	2713	2719	rBV6	24255	48344	1.68%	0.155%
30	18.986	2731	2737	2742	rBV2	109999	239432	8.32%	0.766%
31	19.115	2755	2759	2769	rBV2	149002	224107	7.79%	0.717%
32	19.345	2795	2798	2802	rBV	51898	58713	2.04%	0.188%
33	19.386	2802	2805	2808	rVB	43784	54547	1.90%	0.174%
34	19.562	2829	2835	2840	rBV	2143000	2742460	95.34%	8.771%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270-BM121518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.127	2928	2931	2935	rBV	90845	124482	4.33%	0.398%
36	20.850	3050	3054	3060	rVB2	216842	269560	9.37%	0.862%
37	20.921	3063	3066	3070	rVB	117260	143625	4.99%	0.459%
38	21.127	3096	3101	3105	rBV	1042662	1373356	47.74%	4.392%
39	21.709	3197	3200	3202	rBV2	154633	195026	6.78%	0.624%
40	22.156	3273	3276	3281	rVB3	180737	218816	7.61%	0.700%
41	22.639	3354	3358	3362	rBV2	314426	533724	18.55%	1.707%
42	22.686	3362	3366	3375	rVB	627264	1020381	35.47%	3.263%
43	23.280	3462	3467	3473	rBV	713154	1266188	44.02%	4.050%
44	23.774	3548	3551	3559	rVB	253987	409198	14.23%	1.309%

Sum of corrected areas: 31267457

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
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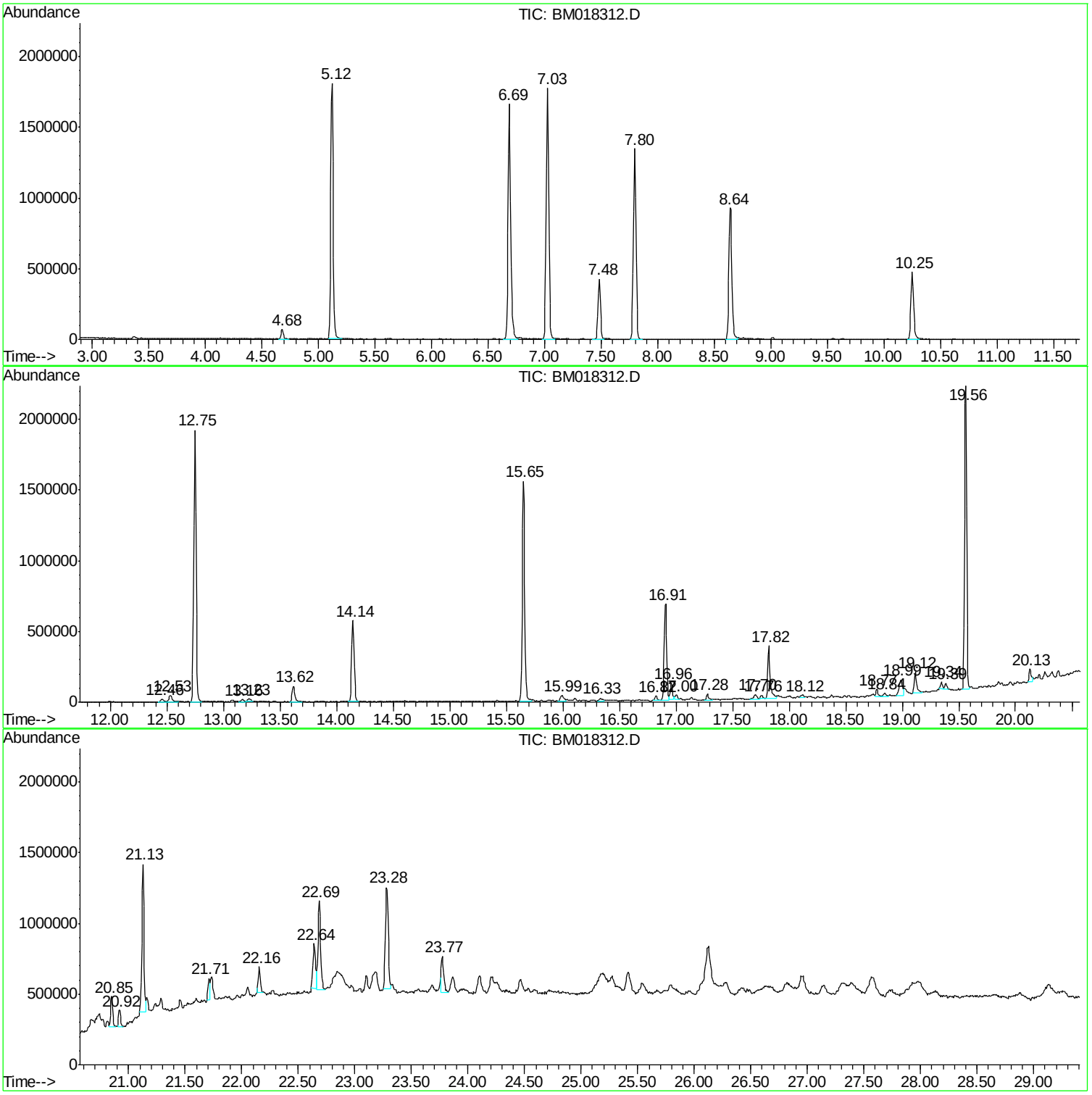
Instrument :
BNA_M
ClientSampleId :
P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

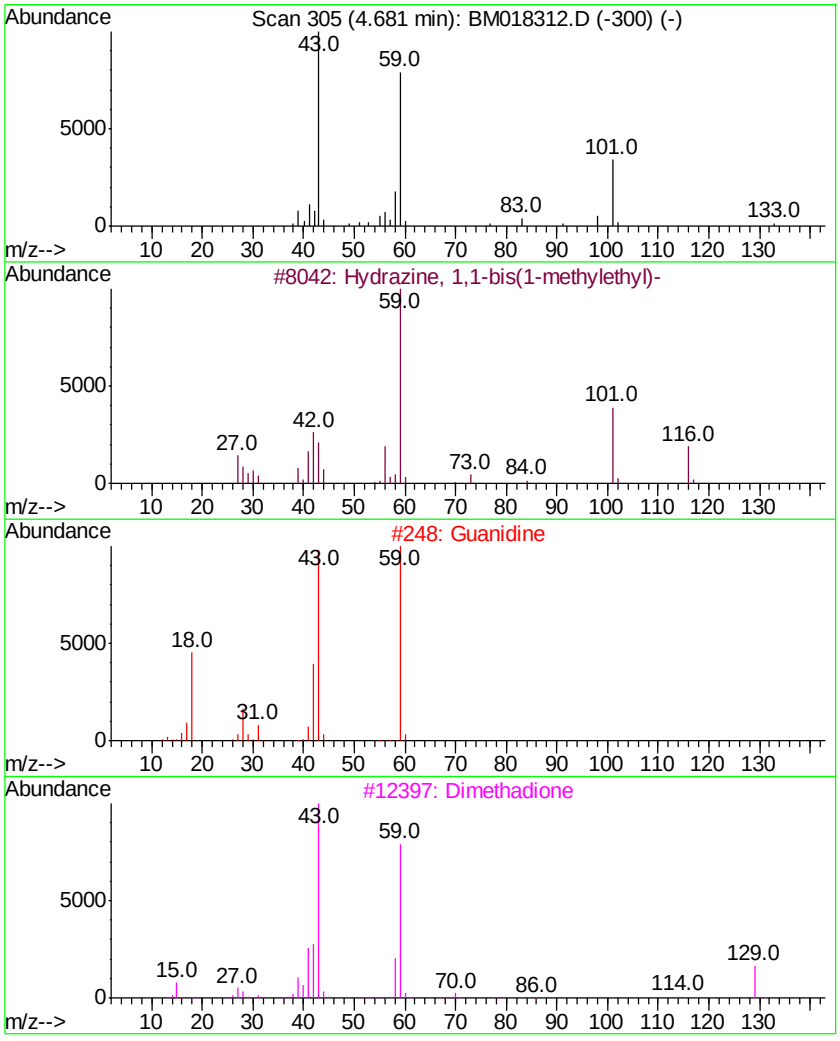
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

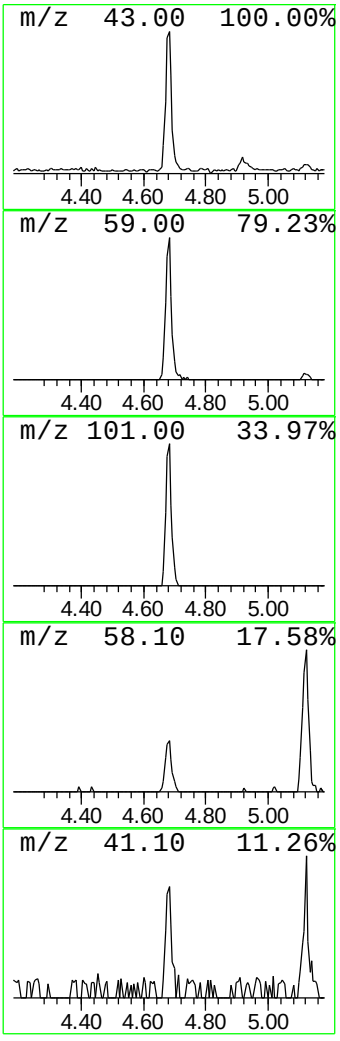
****

Peak Number 1 Hydrazine, 1,1-bis(1-methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.68	2.80 ng	95612	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	53
2	Guanidine	59	CH5N3	000113-00-8	50
3	Dimethadione	129	C5H7NO3	000695-53-4	38
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33





Library Search Compound Report

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Operator : JU/SJ
Sample : J6379-02
Misc :
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Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

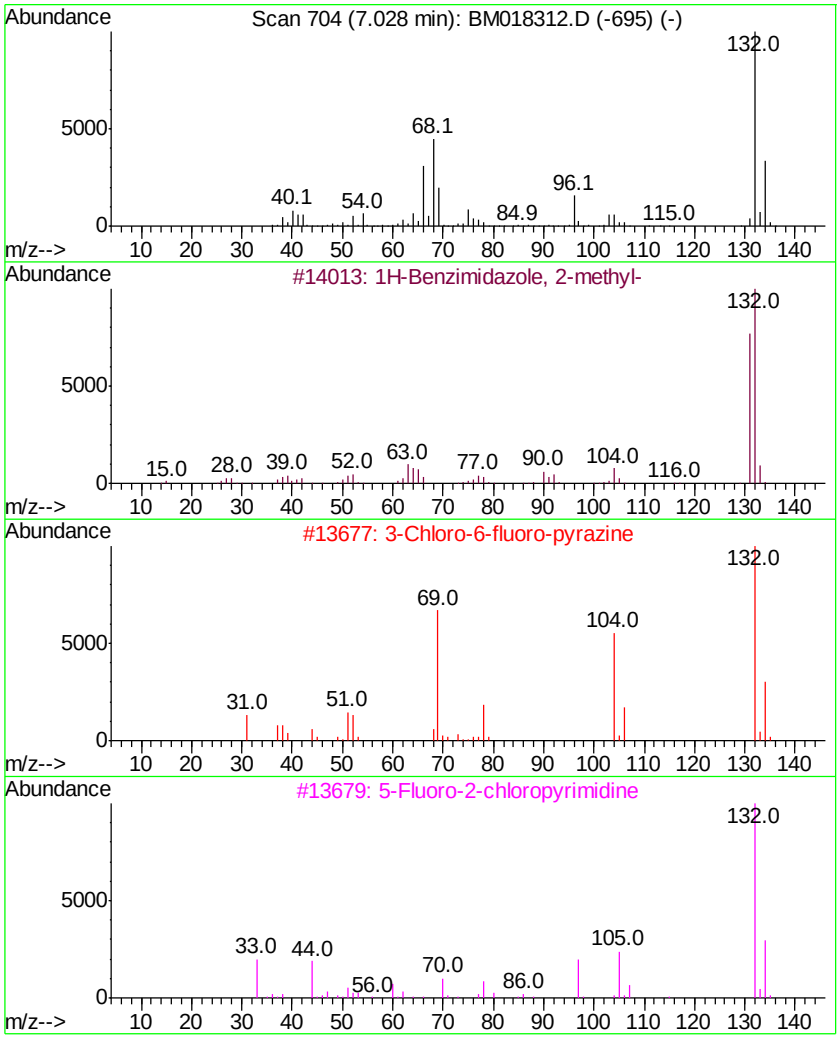
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

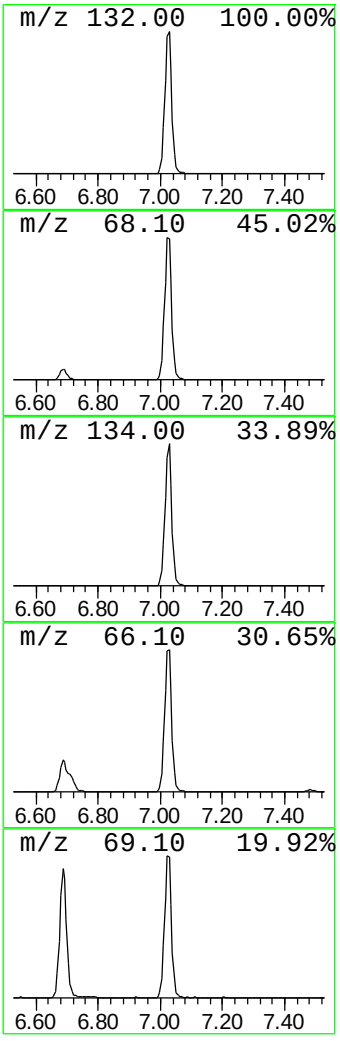
****

Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	82.87 ng	2828240	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

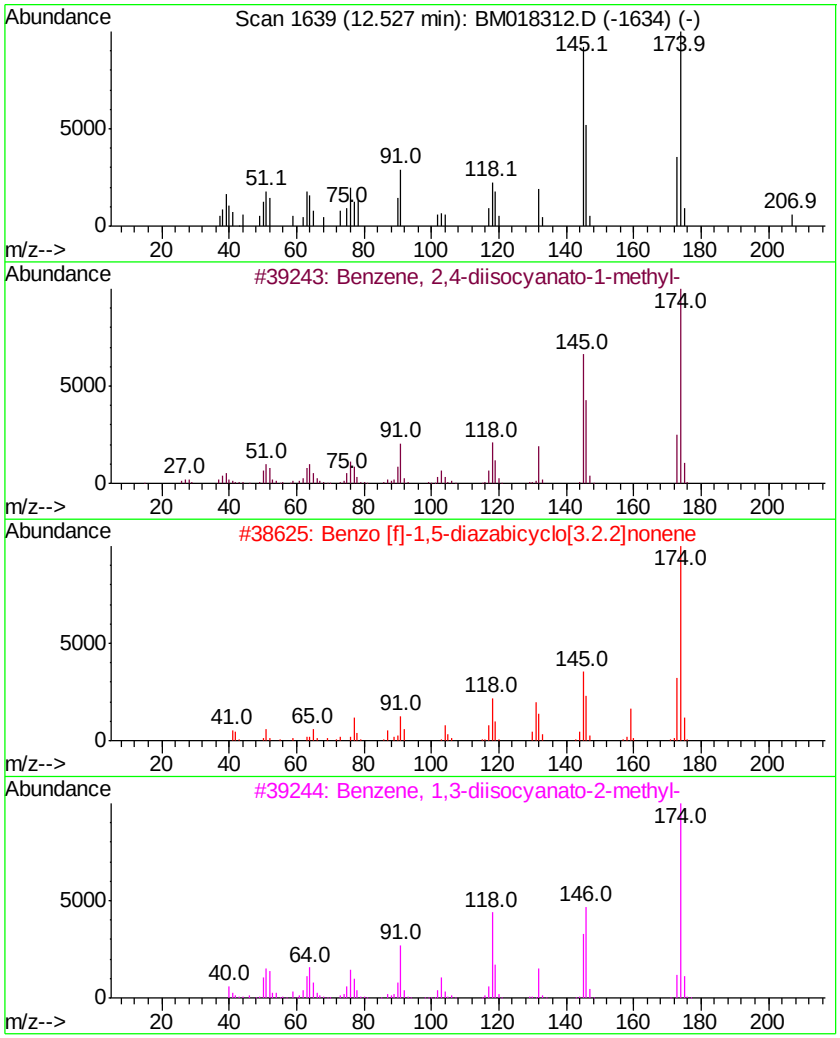
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

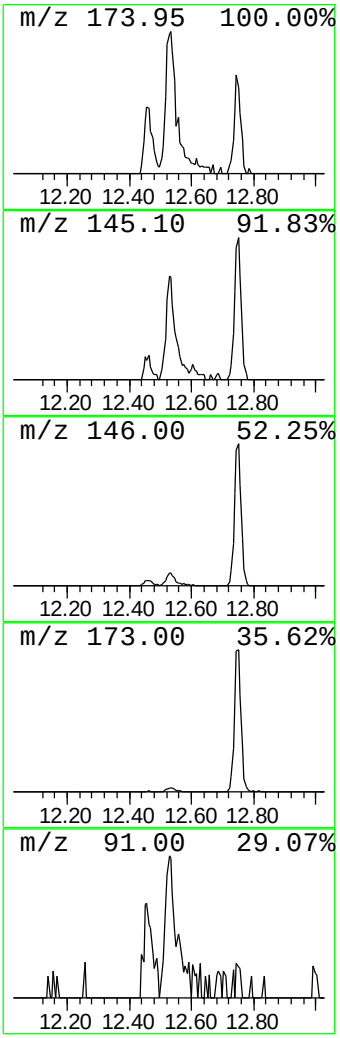
****

Peak Number 4 Benzene, 2,4-diisocyanato-1... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.53	2.18 ng	101611	Acenaphthene-d10	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	94
2	Benzo [f]-1,5-diazabicyclo[3.2.2...	174	C11H14N2	007092-76-4	74
3	Benzene, 1,3-diisocyanato-2-methyl-	174	C9H6N2O2	000091-08-7	64
4	3-Ethyl-1,2-dihydro-2-oxoquinoxa...	174	C10H10N2O	013297-35-3	47
5	1,2-Dihydro-1,3-dimethyl-2-oxoqu...	174	C10H10N2O	003149-25-5	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM121918\
Data File : BM018312.D
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Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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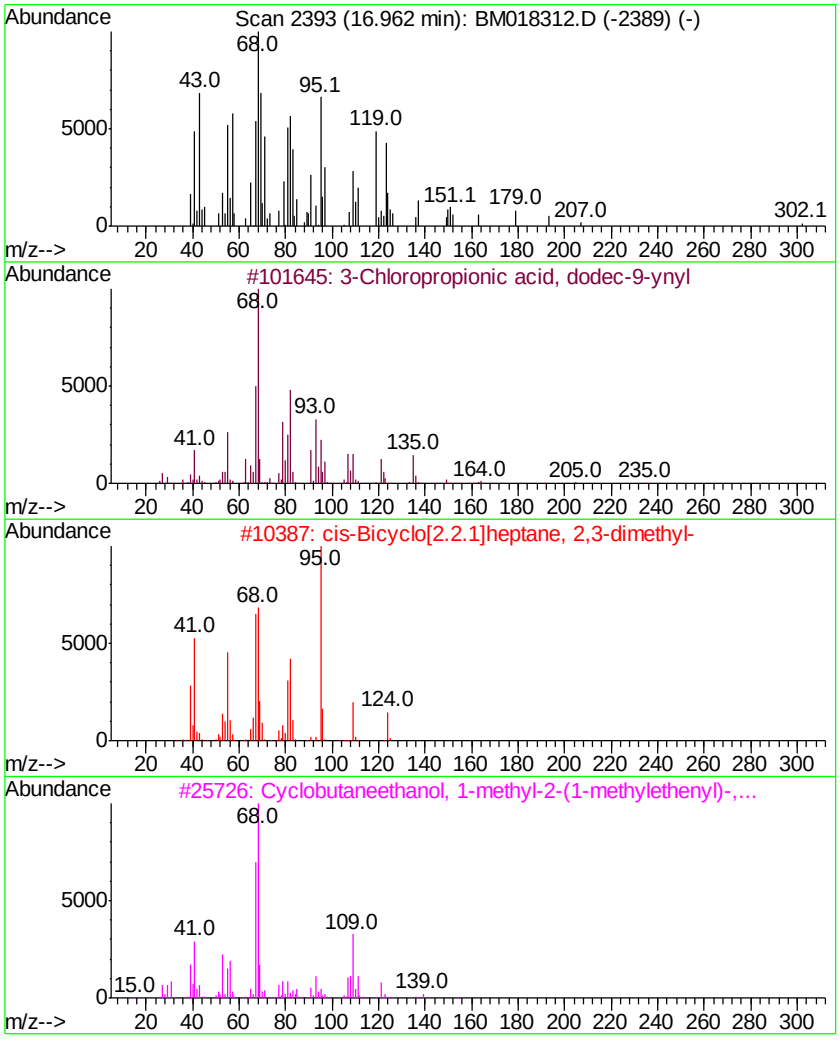
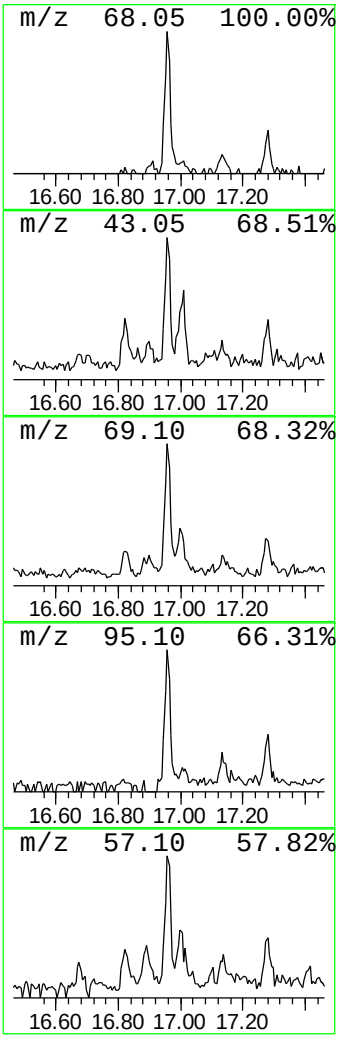
Peak Number 5 unknown16.96 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	3.05 ng	158784	Phenanthrene-d10	16.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloropropionic acid, dodec-9-...	272	C15H25ClO2	1000283-04-9	47
2	cis-Bicyclo[2.2.1]heptane, 2,3-d...	124	C9H16	1000262-02-5	35
3	Cyclobutaneethanol, 1-methyl-2-(...	154	C10H18O	030820-22-5	35
4	3-Nonyne	124	C9H16	020184-89-8	35
5	Cycloheptane, 1-methyl-4-methylene-	124	C9H16	023799-25-9	35





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Instrument : BNA_M
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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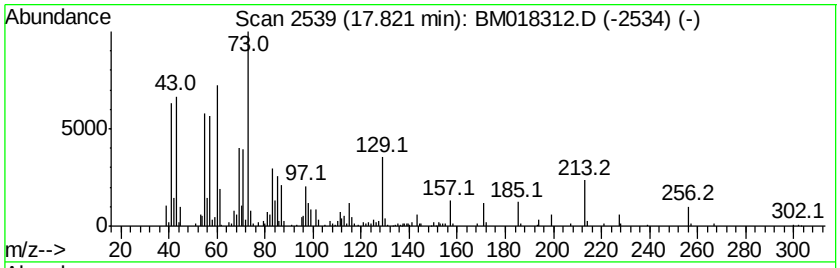
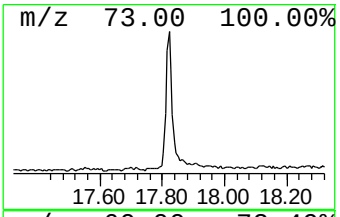
****

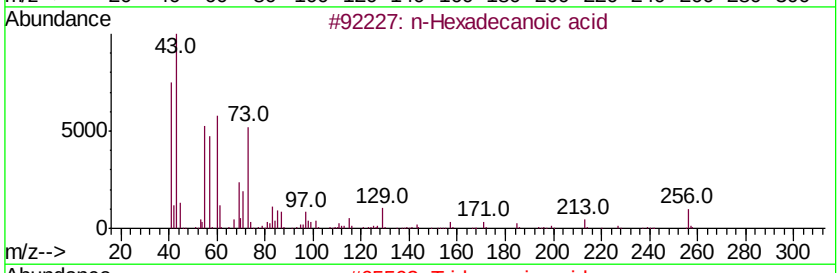
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

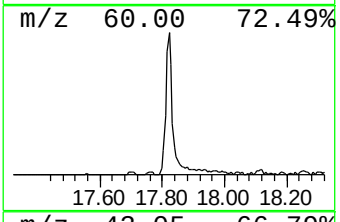
R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	10.76 ng	559147	Phenanthrene-d10	16.90

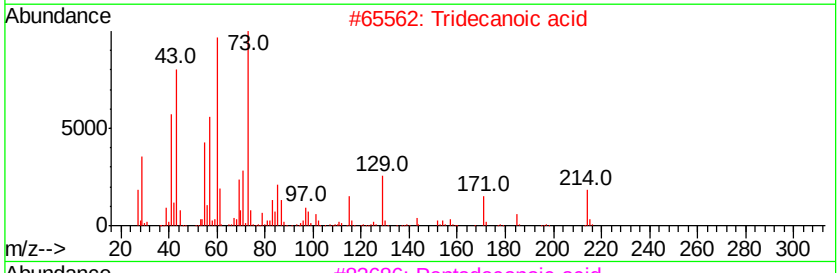
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	30

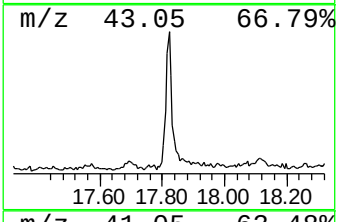


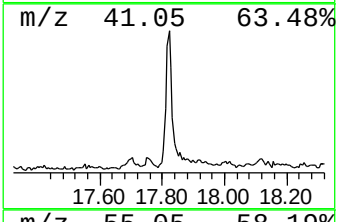


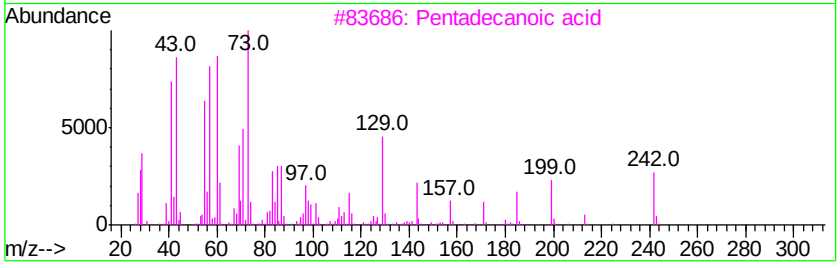


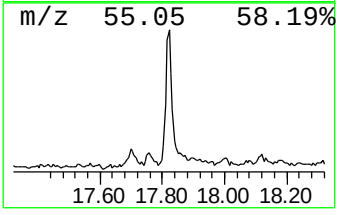












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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

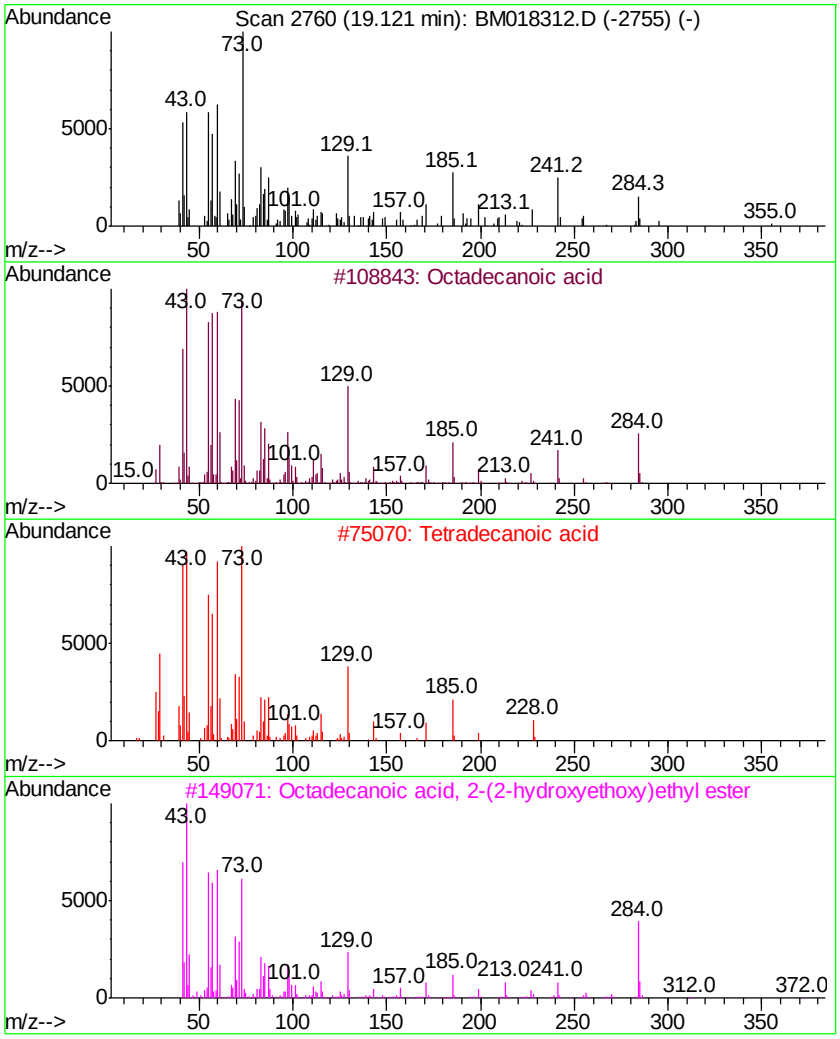
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

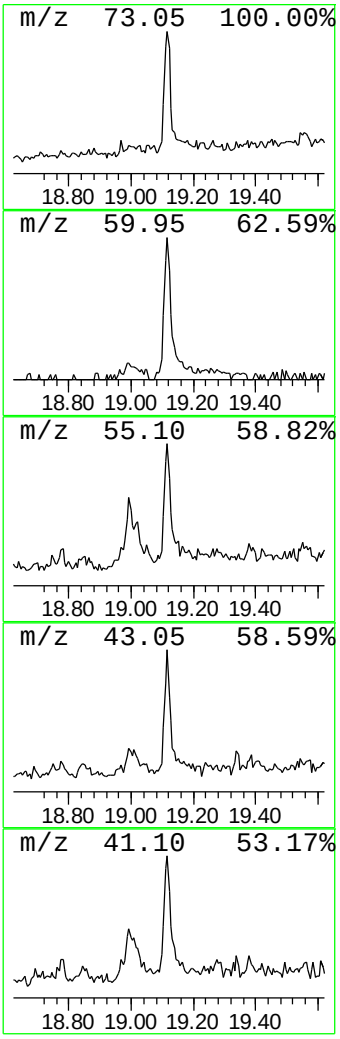
****

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	3.26 ng	224107	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4	Octadecanoic acid, 2-hydroxy-1,3...	625	C39H76O5	000504-40-5	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	55





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Misc :
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Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

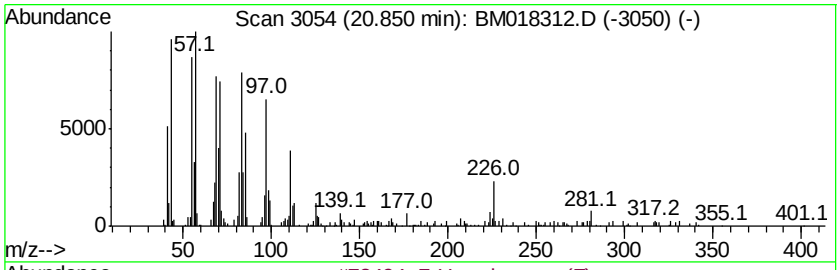
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

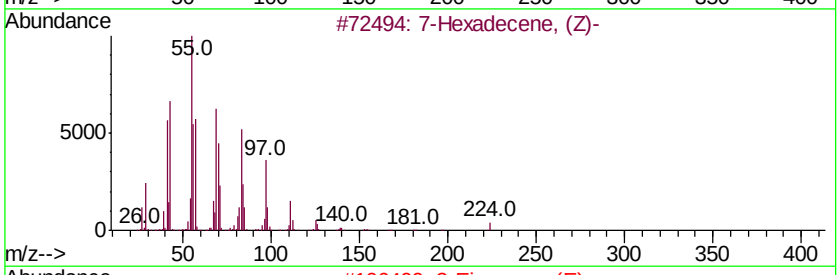
****

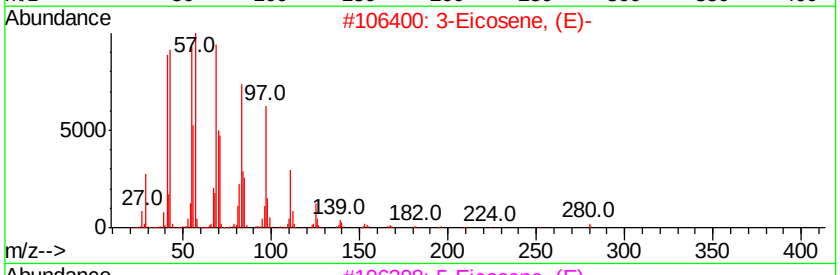
Peak Number 9 7-Hexadecene, (Z)- Concentration Rank 6

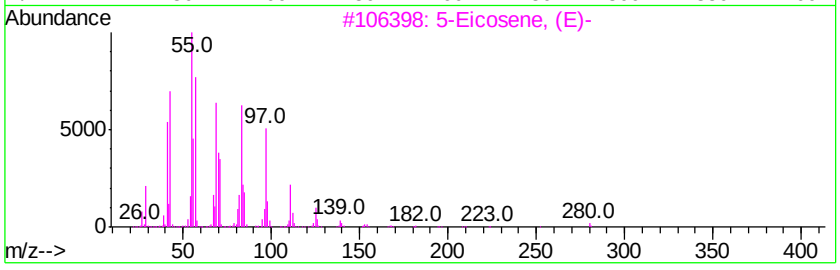
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	3.93 ng	269560	Chrysene-d12	21.13

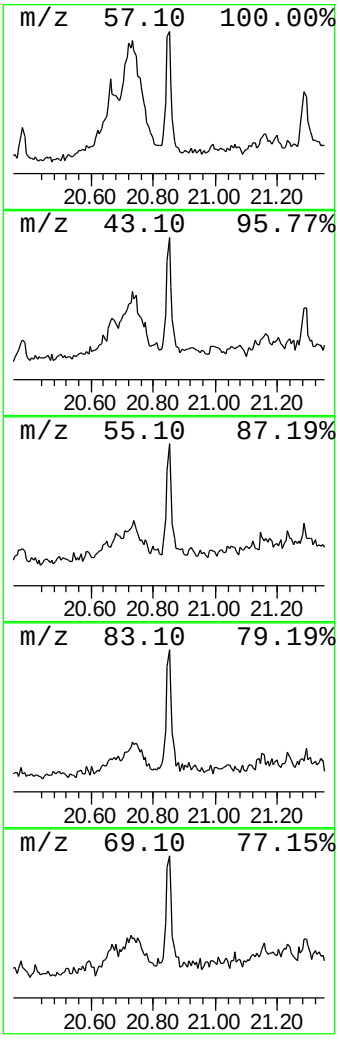
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	93
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	90
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	87
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87
5	Cyclohexadecane	224	C16H32	000295-65-8	86











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Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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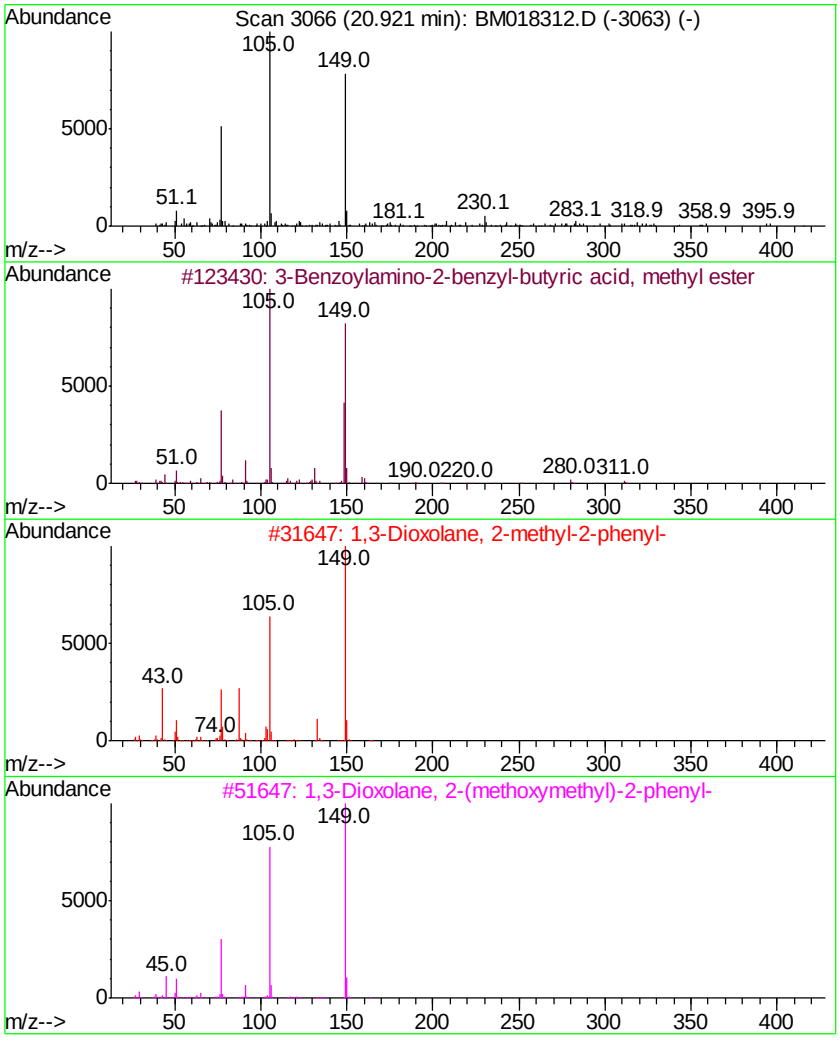
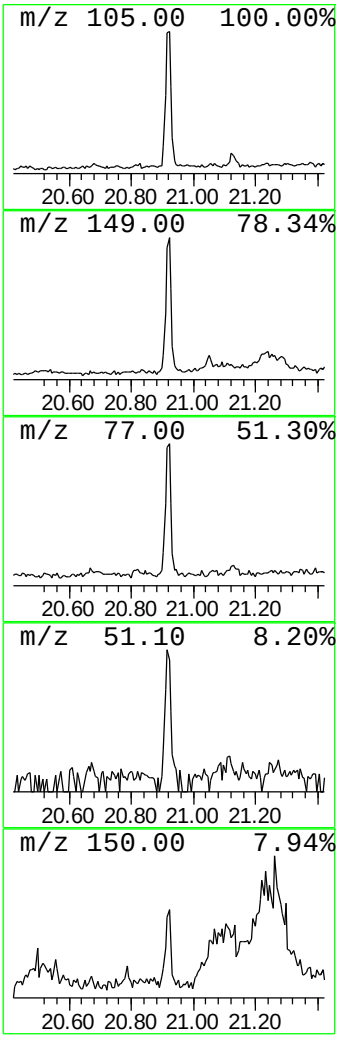
Peak Number 10 3-Benzoylamino-2-benzyl-but... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.92	2.09 ng	143625	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64
2	1,3-Dioxolane, 2-methyl-2-phenyl-	164	C10H12O2	003674-77-9	59
3	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
4	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	50
5	Benzene, 1-isocyanato-3-methoxy-	149	C8H7NO2	018908-07-1	43





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Sample : J6379-02
Misc :
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Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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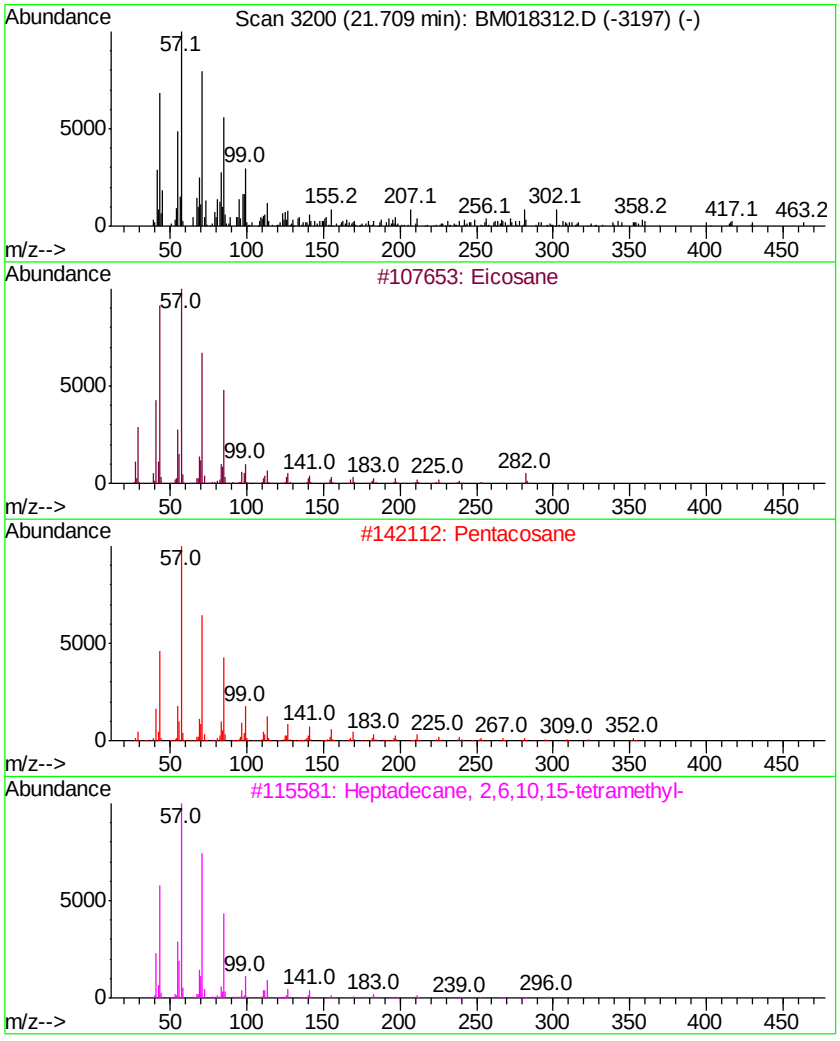
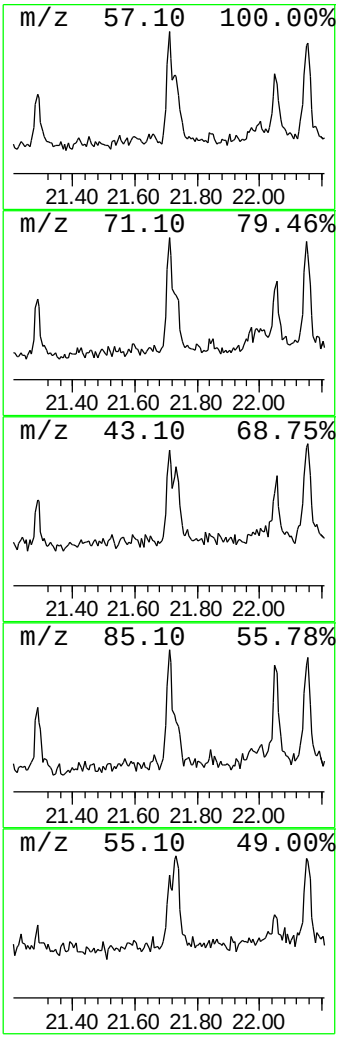
Peak Number 11 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.71	2.84 ng	195026	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Pentacosane	352	C25H52	000629-99-2	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
4	Octadecane	254	C18H38	000593-45-3	90
5	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	81





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Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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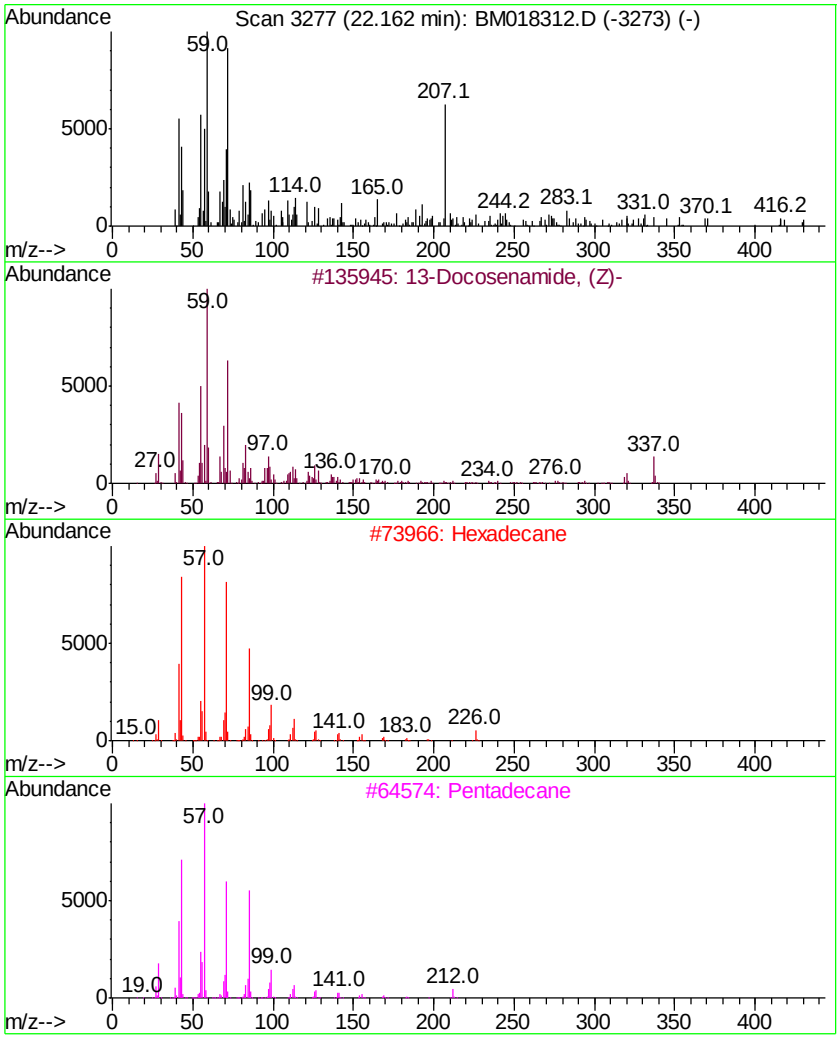
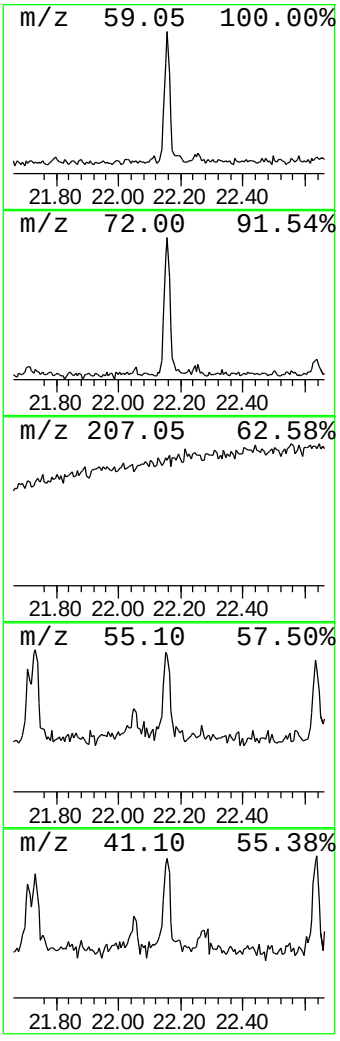
Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.16	3.19 ng	218816	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	53
2	Hexadecane	226	C16H34	000544-76-3	40
3	Pentadecane	212	C15H32	000629-62-9	40
4	3-Tetradecanone	212	C14H28O	000629-23-2	25
5	Octadecanamide	283	C18H37NO	000124-26-5	25





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Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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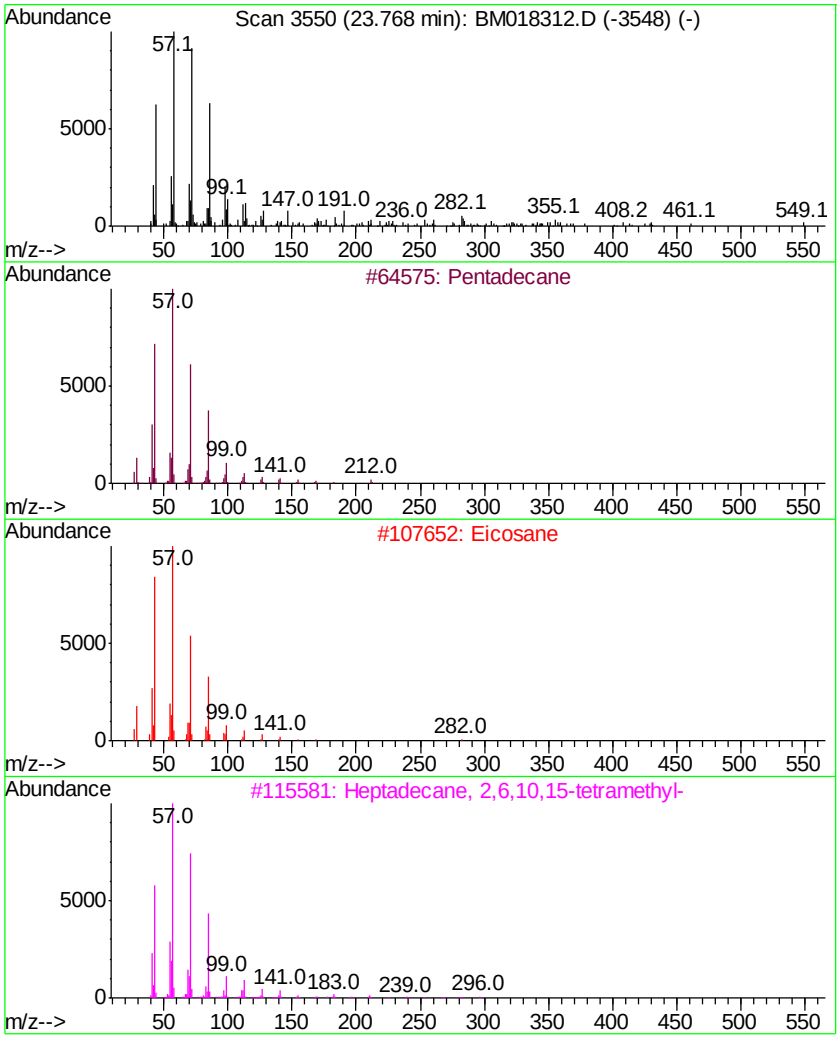
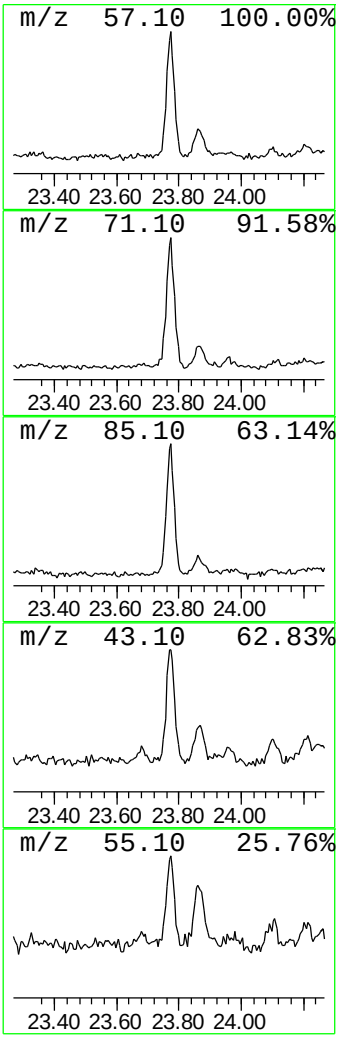
Peak Number 13 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.77	6.46 ng	409198	Perylene-d12	23.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Eicosane	282	C20H42	000112-95-8	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	89
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	76
5	Tetratetracontane	619	C44H90	007098-22-8	68





Tentatively Identified Compound (LSC) summary

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Data File : BM018312.D
Acq On : 20 Dec 2018 00:37
Operator : JU/SJ
Sample : J6379-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : P001-SS003-0006-01

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Hydrazine, 1,1-bi...	4.68	2.8	ng	95612	1	7.48	682613	20.0
unknown7.03	7.03	82.9	ng	2828240	1	7.48	682613	20.0
Benzene, 2,4-diis...	12.53	2.2	ng	101611	3	14.14	932616	20.0
unknown16.96	16.96	3.0	ng	158784	4	16.90	1039770	20.0
n-Hexadecanoic acid	17.82	10.8	ng	559147	4	16.90	1039770	20.0
Octadecanoic acid	19.12	3.3	ng	224107	5	21.13	1373360	20.0
7-Hexadecene, (Z)-	20.85	3.9	ng	269560	5	21.13	1373360	20.0
3-Benzoylamino-2-...	20.92	2.1	ng	143625	5	21.13	1373360	20.0
Eicosane	21.71	2.8	ng	195026	5	21.13	1373360	20.0
13-Docosenamide, ...	22.16	3.2	ng	218816	5	21.13	1373360	20.0
Pentadecane	23.77	6.5	ng	409198	6	23.28	1266190	20.0