LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP120921\
Data File : BP008331.D
Acq On : 10 Dec 2021 02:11
Operator : CG/JU
Sample : M4967-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-8S

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_P\Methods\8270E-BP112521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	13	rVB	183714	211697	6.00%	1.134%
2	3.264	42	47	57	rBV	27137	47869	1.36%	0.256%
3	3.970	162	167	173	rVB	26925	40139	1.14%	0.215%
4	4.522	257	261	267	rVB	28616	38592	1.09%	0.207%
5	4.899	320	325	334	rVB2	34462	50726	1.44%	0.272%
6	5.364	398	404	410	rVV	1138780	1769907	50.17%	9.479%
7	5.411	410	412	421	rVB	65504	119753	3.39%	0.641%
8	5.781	469	475	481	rVB	25215	41394	1.17%	0.222%
9	6.958	666	675	685	rBV	1009565	1816575	51.49%	9.729%
10	7.763	805	812	820	rVB	253229	400064	11.34%	2.143%
11	8.928	1003	1010	1026	rVB	651144	1123720	31.85%	6.018%
12	10.563	1280	1288	1303	rBV	282796	528726	14.99%	2.832%
13	13.034	1701	1708	1734	rBV	1442193	2225222	63.08%	11.918%
14	14.416	1937	1943	1959	rVB	417939	679878	19.27%	3.641%
15	15.845	2180	2186	2192	rBV2	87389	116194	3.29%	0.622%
16	15.922	2192	2199	2219	rBV	1064144	1825616	51.75%	9.778%
17	17.181	2407	2413	2423	rBV	543253	838773	23.78%	4.492%
18	17.310	2430	2435	2443	rVB5	46146	73475	2.08%	0.394%
19	17.481	2460	2464	2472	rVB2	18899	37327	1.06%	0.200%
20	17.845	2521	2526	2533	rVB2	31729	57717	1.64%	0.309%
21	18.081	2562	2566	2573	rBV	68030	109281	3.10%	0.585%
22	18.151	2574	2578	2582	rVB	33250	43315	1.23%	0.232%
23	18.975	2715	2718	2725	rVB3	25577	43306	1.23%	0.232%
24	19.204	2755	2757	2764	rVB4	25132	40991	1.16%	0.220%
25	19.757	2845	2851	2862	rVB	2885363	3527827	100.00%	18.894%
26	20.504	2975	2978	2981	rVB2	66956	67241	1.91%	0.360%
27	21.004	3059	3063	3072	rVB	142297	236778	6.71%	1.268%
28	21.198	3093	3096	3102	rVB	140930	155878	4.42%	0.835%
29	21.292	3107	3112	3124	rVV	772853	1122439	31.82%	6.012%
30	22.174	3258	3262	3270	rVB2	97660	141026	4.00%	0.755%
31	23.674	3511	3517	3528	rVB2	538261	1139922	32.31%	6.105%

Sum of corrected areas: 18671368

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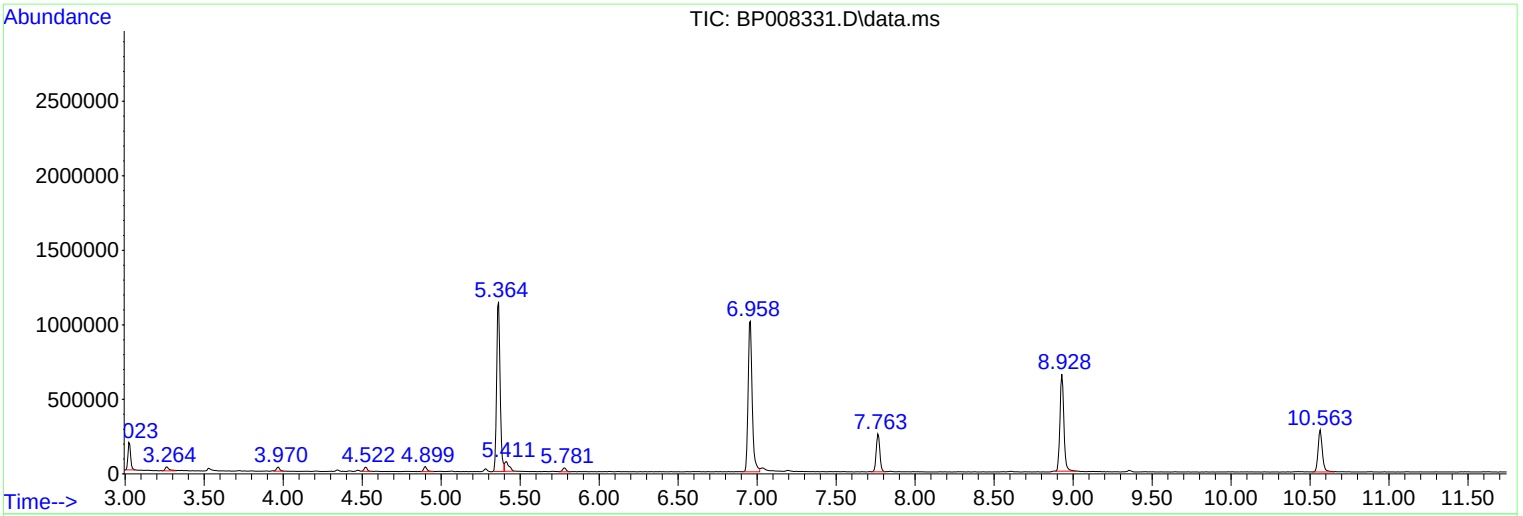
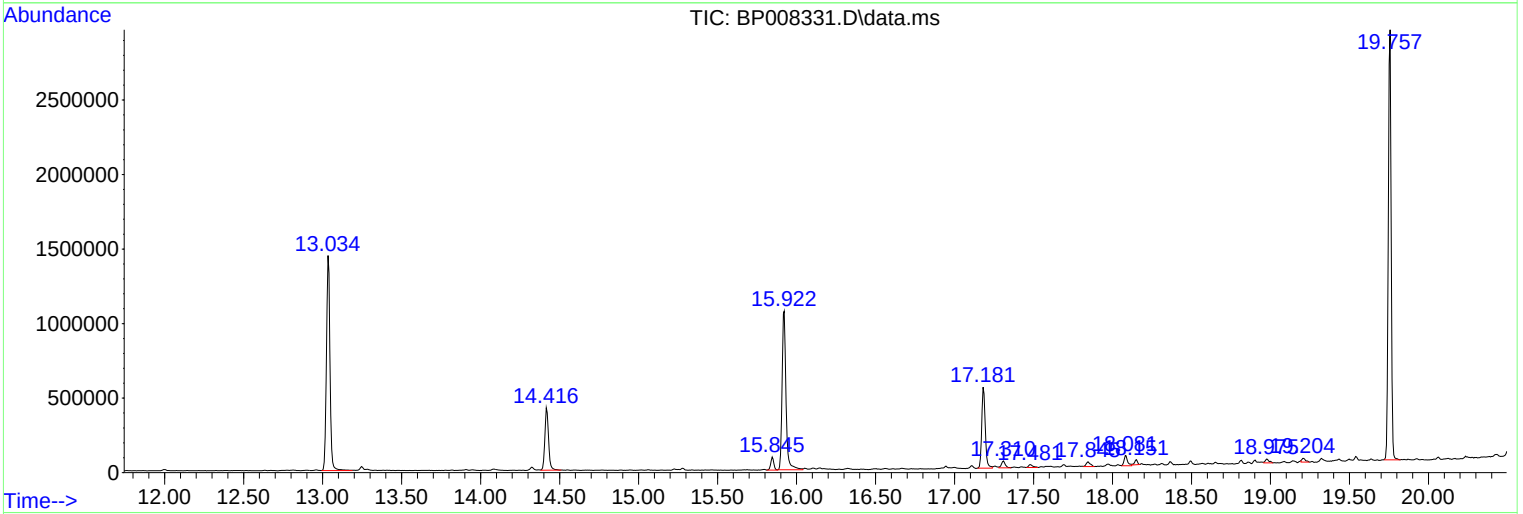
Misc :
ALS Vial : 20 Sample Multiplier: 1

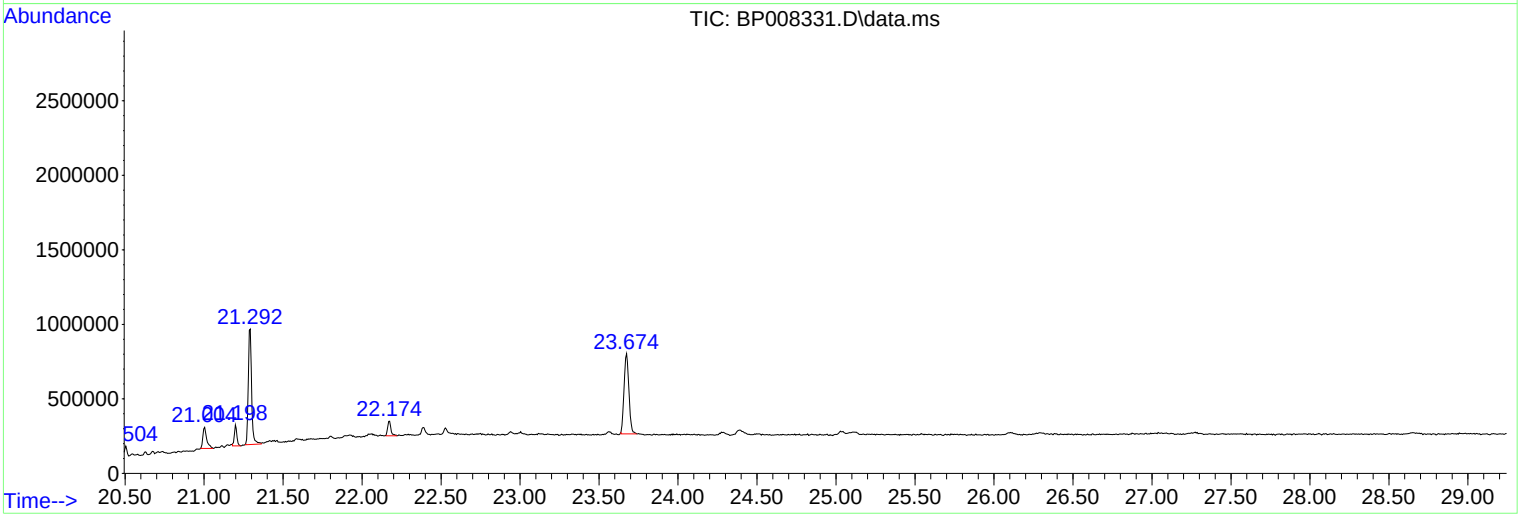
Instrument :
BNA_P
ClientSampleId :
TP-8S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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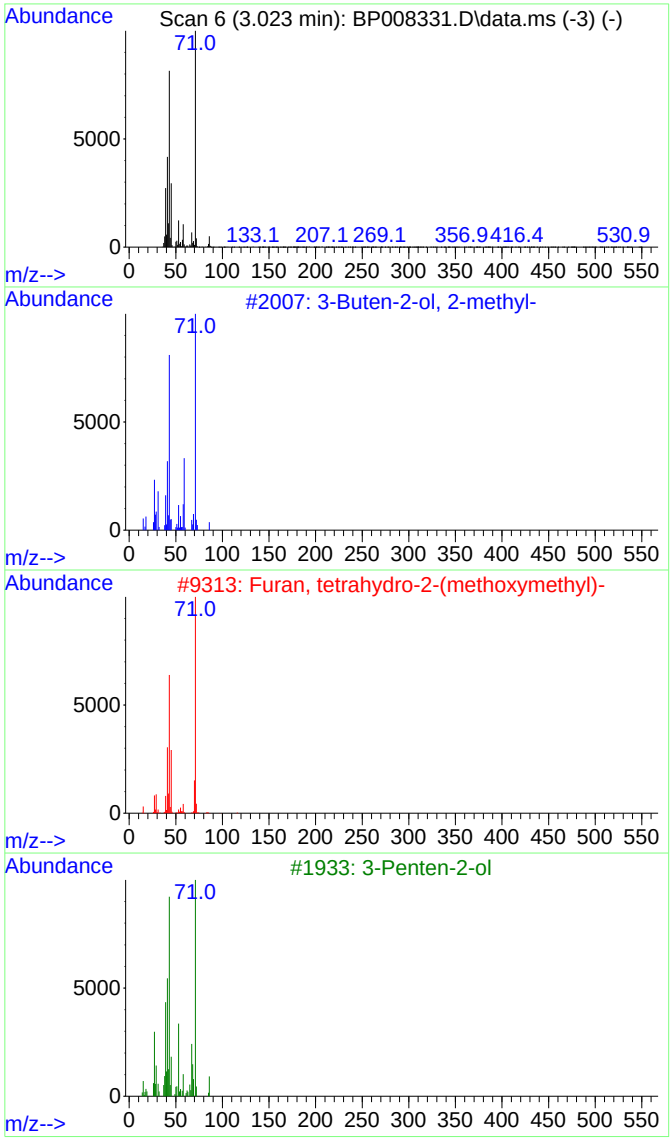
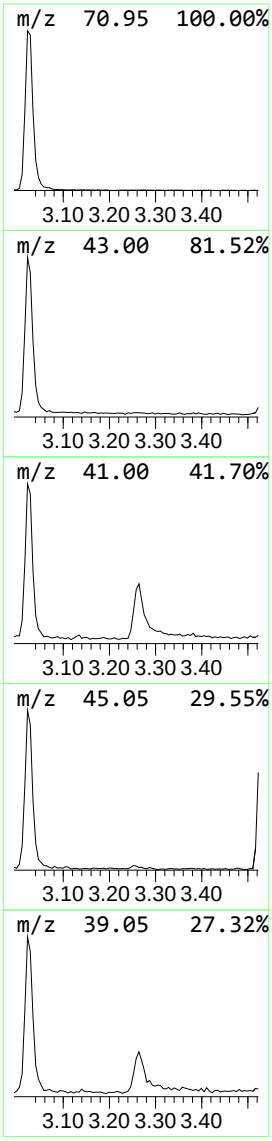
****

Peak Number 1 3-Buten-2-ol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.023	10.58 ng	211697	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	72
2	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
3	3-Penten-2-ol	86	C5H10O	001569-50-2	72
4	Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	53
5	Hexanoic acid, 3-oxo-, ethyl ester	158	C8H14O3	003249-68-1	53





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Data File : BP008331.D
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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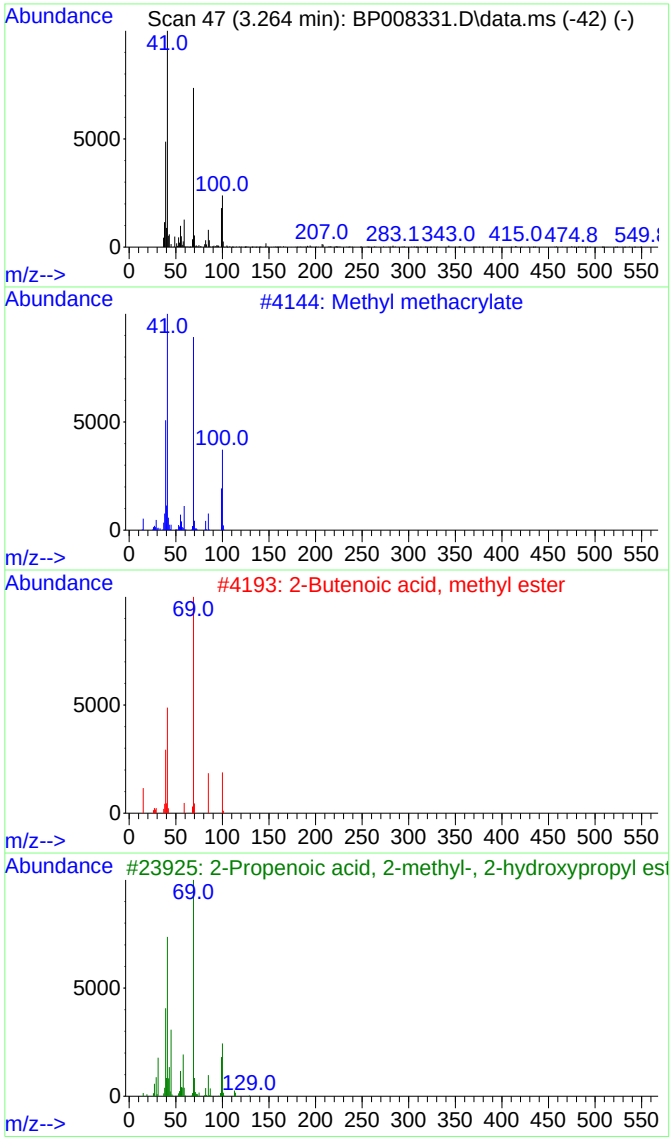
TIC Integration Parameters: LSCINT.P

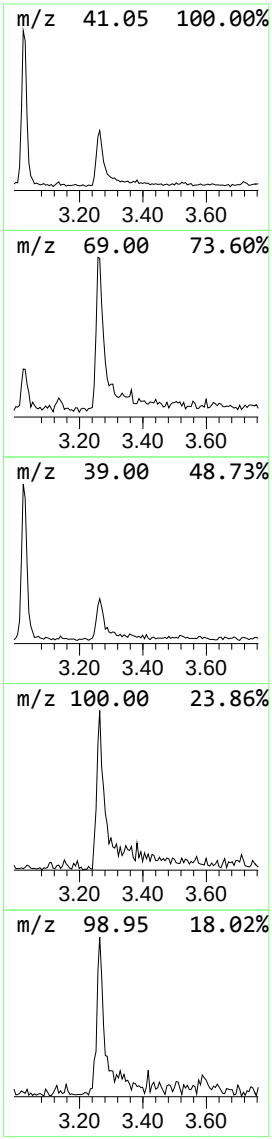
****

Peak Number 2 Methyl methacrylate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.264	2.39 ng	47869	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl methacrylate	100	C5H8O2	000080-62-6	93
2	2-Butenoic acid, methyl ester	100	C5H8O2	018707-60-3	59
3	2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	56
4	2-Propenoic acid, 2-methyl-, 3-h...	144	C7H12O3	002761-09-3	56
5	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	50





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TP-8S

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

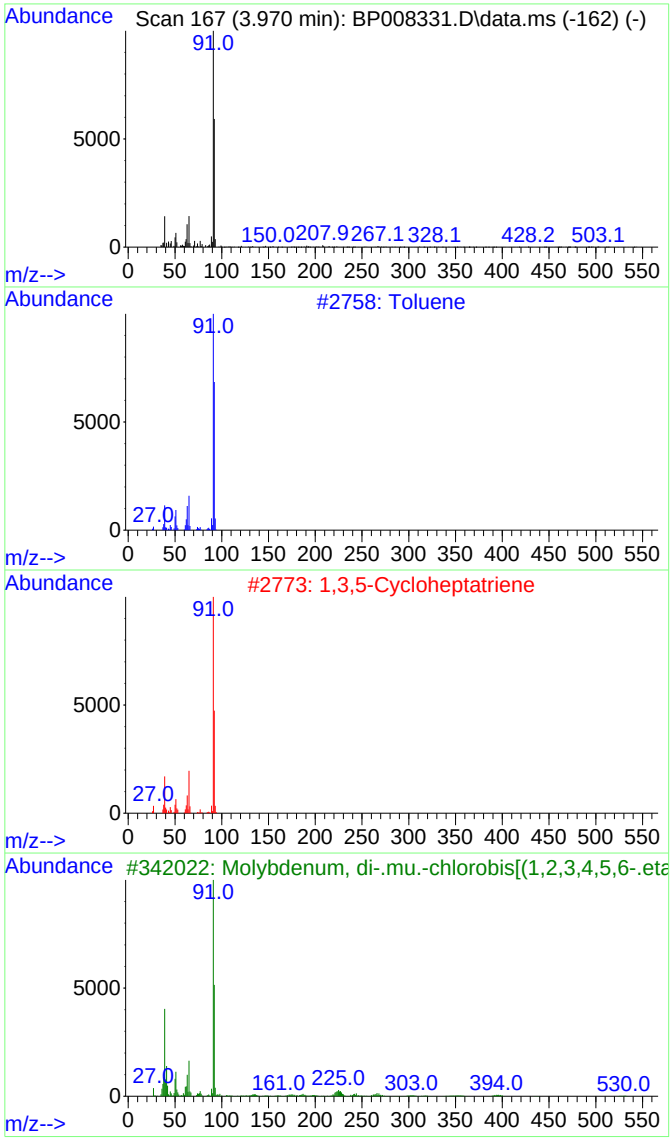
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

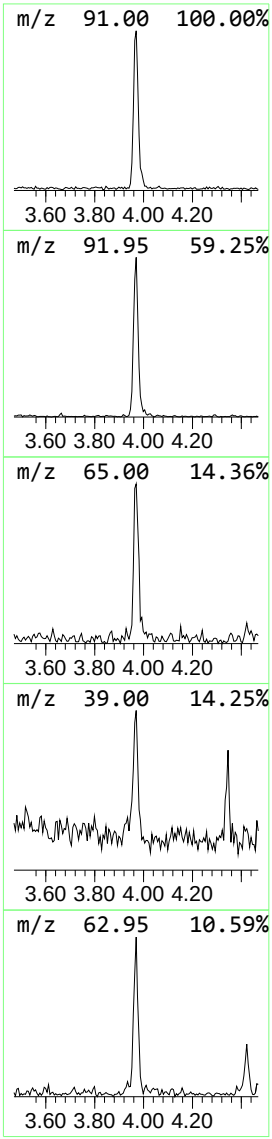
****

Peak Number 3 1,3,5-Cycloheptatriene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.970	2.01 ng	40139	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Toluene	92	C7H8	000108-88-3	93
2	1,3,5-Cycloheptatriene	92	C7H8	000544-25-2	90
3	Molybdenum, di-.mu.-chlorobis[(1...	532	C20H26Cl2Mo2	035625-66-2	78
4	Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	64
5	Benzeneacetamide	135	C8H9NO	000103-81-1	64





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Instrument :
BNA_P
ClientSampleId :
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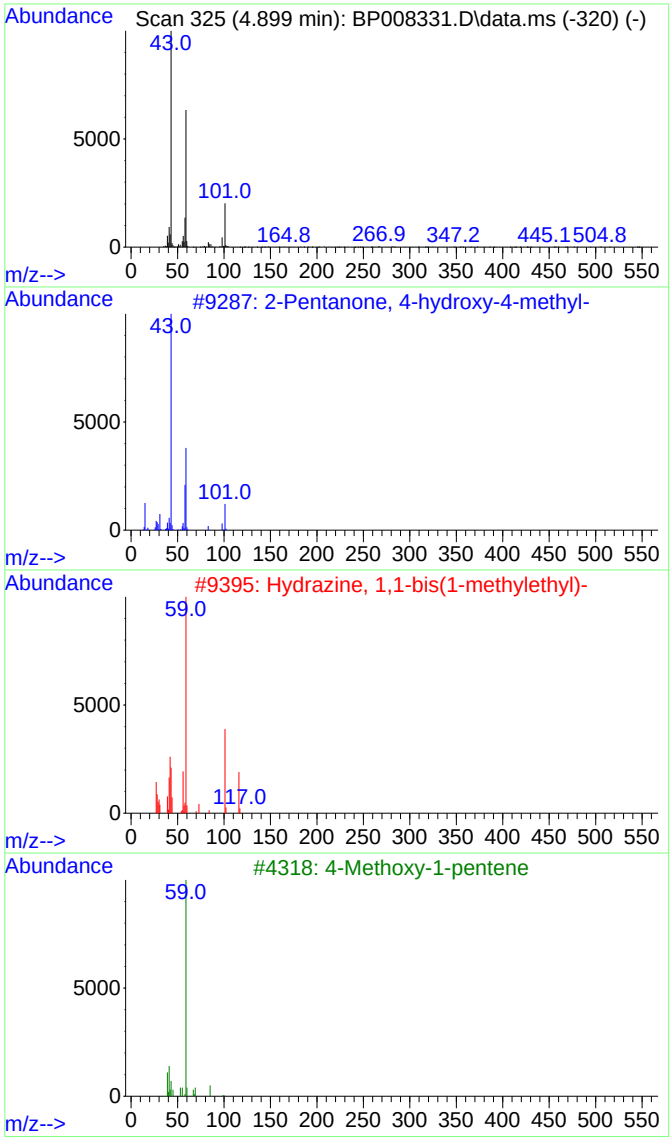
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP112521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

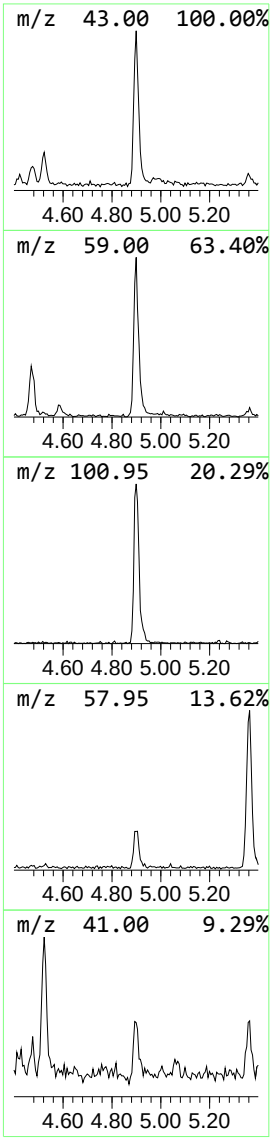
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.899	2.54 ng	50726	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	35
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	25





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Instrument :
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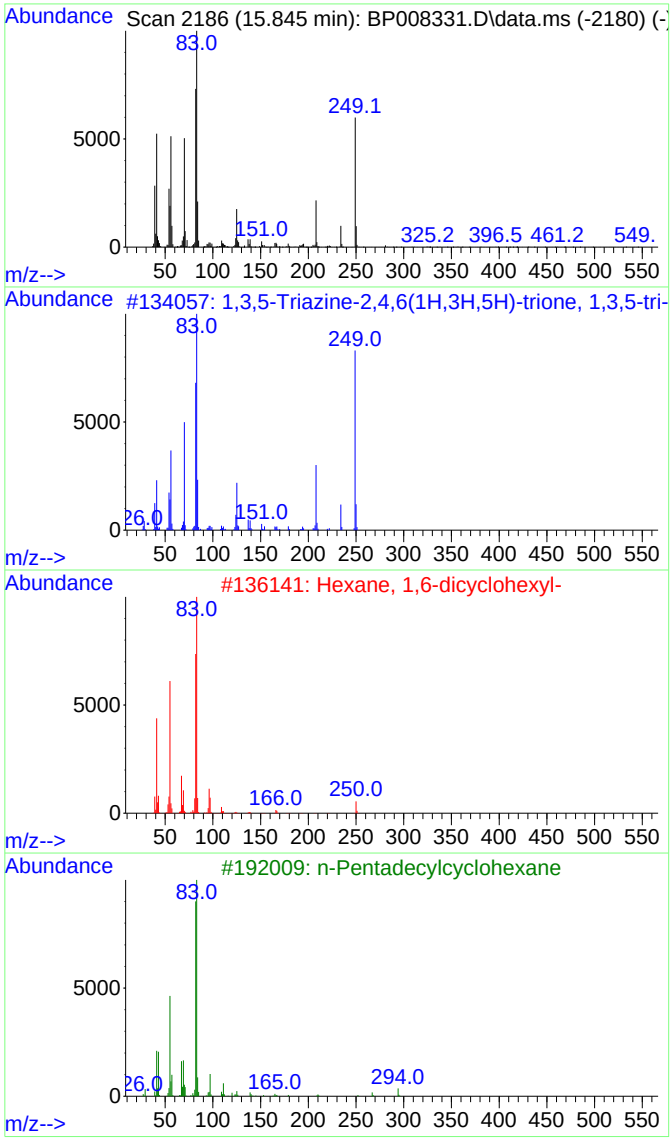
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

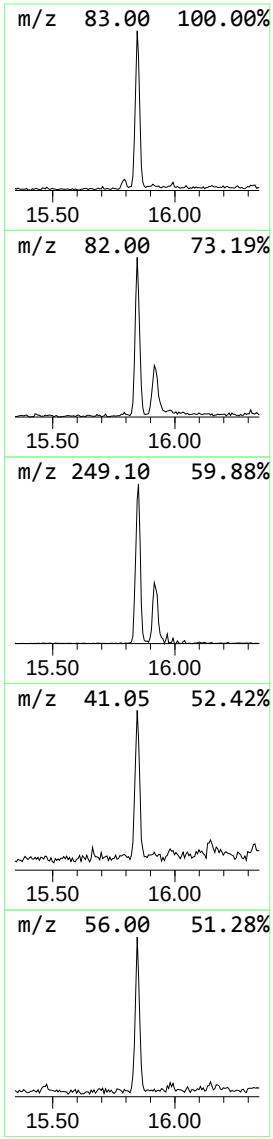
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.845	2.77 ng	116194	Phenanthrene-d10	17.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	97
2	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	32
3	n-Pentadecylcyclohexane	294	C21H42	006006-95-7	32
4	Azetidine, 2-methyl-1-[3,3,3-tri...	249	C8H9F6NO	050837-79-1	27
5	Succinic acid, cis-hex-3-enyl do...	368	C22H40O4	1000353-41-4	14





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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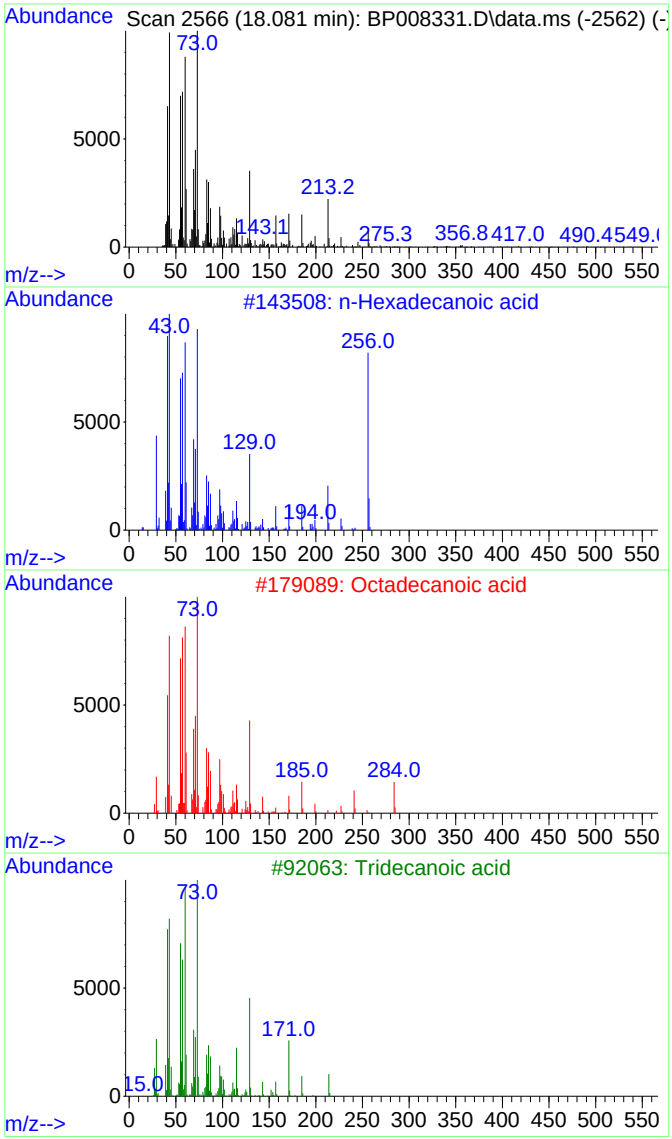
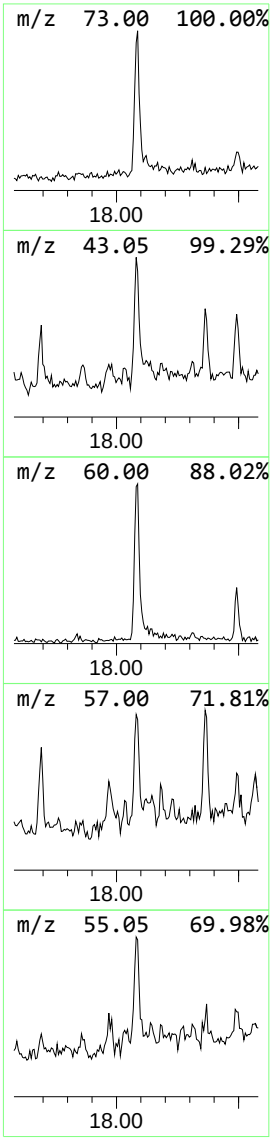
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.081	2.61 ng	109281	Phenanthrene-d10	17.181

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53





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TIC Library : C:\Database\NIST20.L
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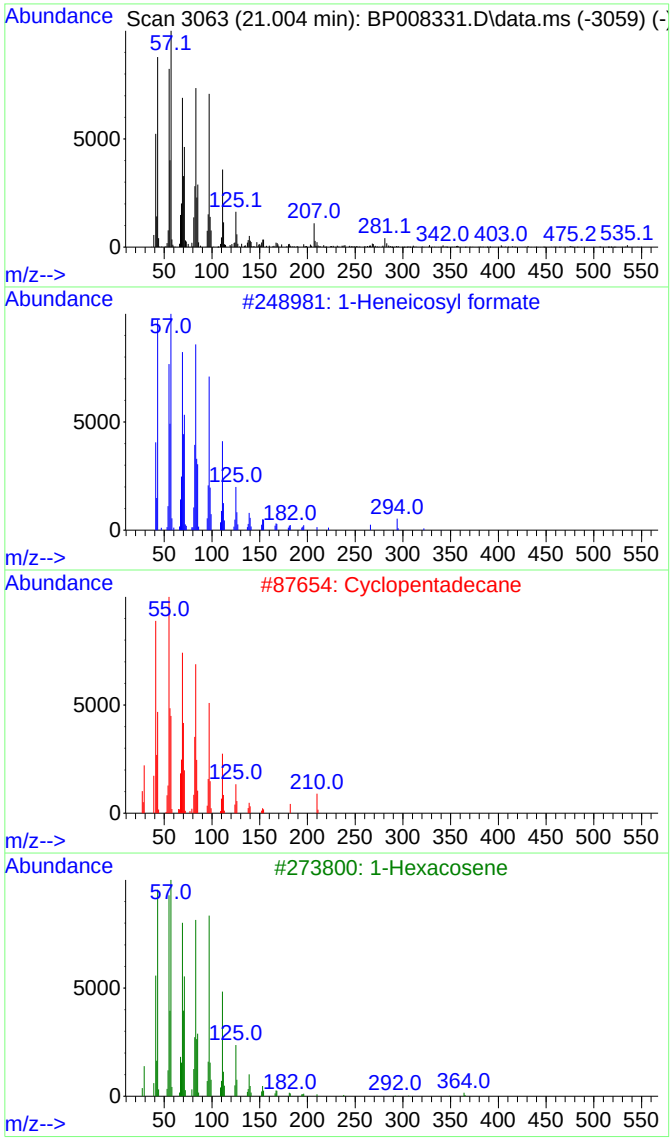
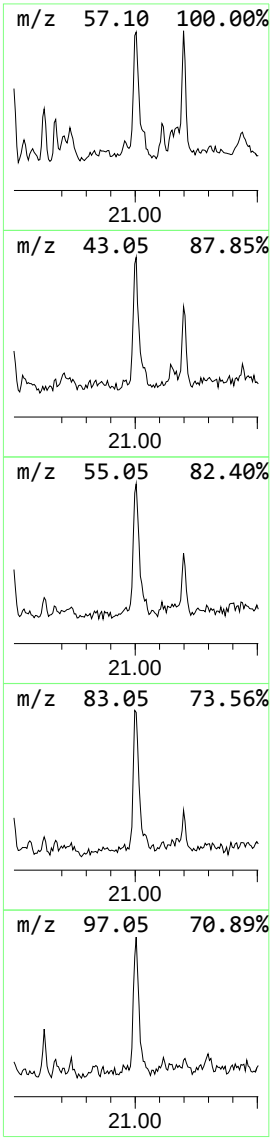
****

Peak Number 8 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.004	4.22 ng	236778	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptacos-1-ene	378	C27H54	015306-27-1	93





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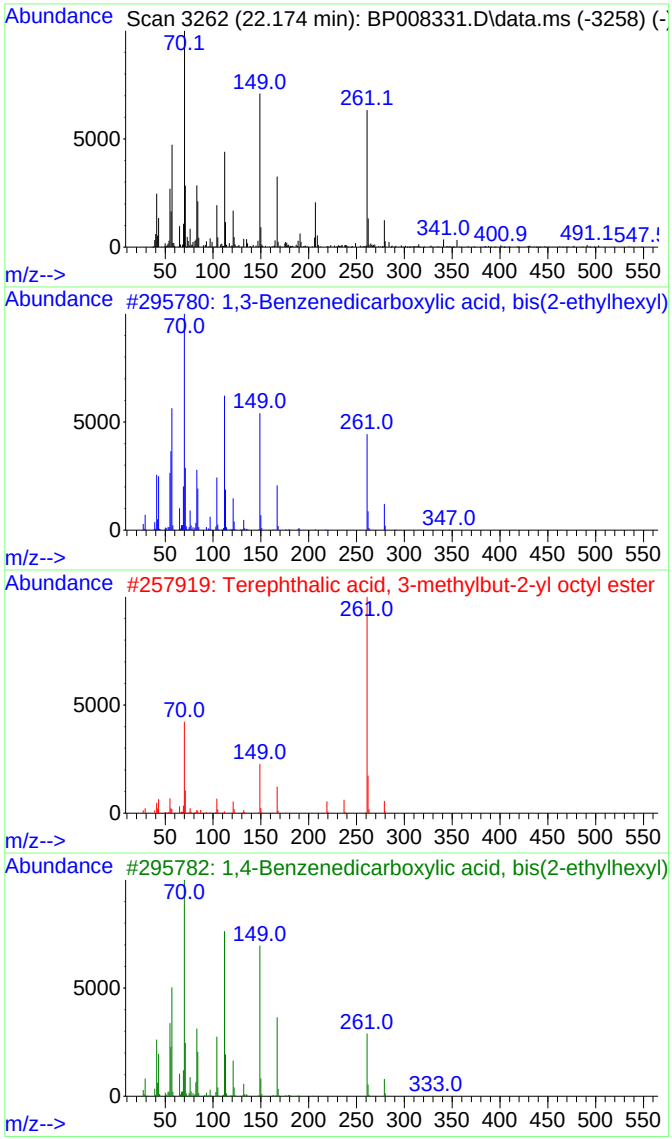
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

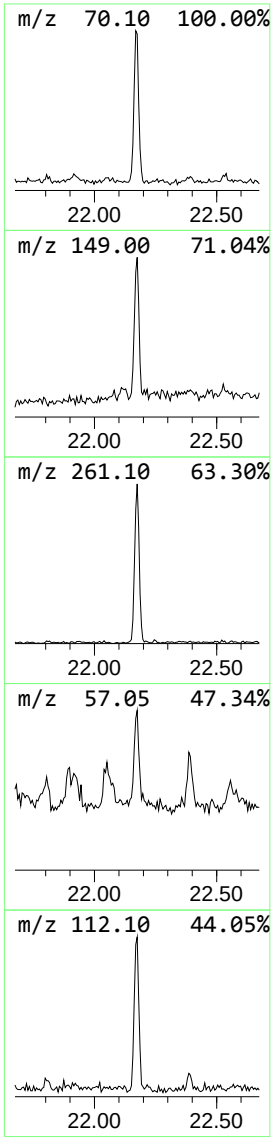
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,3-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.174	2.51 ng	141026	Chrysene-d12	21.292

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
2	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	58
3	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	49
4	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	38
5	N-(4-Nitrophenyl)-2-pyrrolidinec...	277	C13H15N3O4	1286682-74-3	27





Tentatively Identified Compound (LSC) summary

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Data File : BP008331.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
3-Buten-2-ol, 2...	3.023	10.6	ng	211697	1	7.763	400064	20.0
Methyl methacry...	3.264	2.4	ng	47869	1	7.763	400064	20.0
1,3,5-Cyclohept...	3.970	2.0	ng	40139	1	7.763	400064	20.0
2-Pentanone, 4-...	4.899	2.5	ng	50726	1	7.763	400064	20.0
1,3,5-Triazine-...	15.845	2.8	ng	116194	4	17.181	838773	20.0
n-Hexadecanoic ...	18.081	2.6	ng	109281	4	17.181	838773	20.0
1-Heneicosyl fo...	21.004	4.2	ng	236778	5	21.292	1122440	20.0
1,3-Benzenedica...	22.174	2.5	ng	141026	5	21.292	1122440	20.0