LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008100.D
Acq On : 23 Nov 2021 17:21
Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

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-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008100.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	13	rBV	880007	1069955	2.18%	1.120%
2	4.946	328	333	345	rVB	384203	537464	1.10%	0.563%
3	5.411	405	412	424	rBV	2062204	3020652	6.15%	3.162%
4	6.999	673	682	696	rBV	1828374	3062269	6.24%	3.206%
5	7.822	814	822	829	rBV	544196	895109	1.82%	0.937%
6	8.981	1012	1019	1026	rBV	1156766	1895952	3.86%	1.985%
7	10.616	1289	1297	1307	rVB	621051	1123366	2.29%	1.176%
8	13.087	1709	1717	1724	rBV	2028449	3443062	7.01%	3.605%
9	13.251	1741	1745	1754	rBV3	346195	633660	1.29%	0.663%
10	13.887	1849	1853	1858	rBV	945579	1419165	2.89%	1.486%
11	13.963	1862	1866	1869	rVB2	831694	1102509	2.25%	1.154%
12	14.210	1904	1908	1912	rBV4	493499	909171	1.85%	0.952%
13	14.298	1919	1923	1931	rVB	1577929	2619055	5.34%	2.742%
14	14.375	1931	1936	1941	rBV3	450226	955516	1.95%	1.000%
15	14.439	1942	1947	1949	rBV3	817329	1428192	2.91%	1.495%
16	15.004	2039	2043	2049	rBV2	1081727	1675213	3.41%	1.754%
17	15.263	2083	2087	2091	rVB2	1180988	1599802	3.26%	1.675%
18	15.745	2166	2169	2175	rVB	1546279	2324638	4.74%	2.434%
19	15.957	2201	2205	2213	rBV4	1230572	2585641	5.27%	2.707%
20	16.233	2248	2252	2262	rVB	3297946	5209689	10.61%	5.454%
21	17.057	2389	2392	2400	rVB	2271262	3636245	7.41%	3.807%
22	19.798	2855	2858	2868	rVB	2744507	3737013	7.61%	3.912%
23	23.721	3520	3525	3532	rVB2	790952	1554829	3.17%	1.628%
24	27.815	4199	4221	4240	rVB	10217516	49082208	100.00%	51.384%

Sum of corrected areas: 95520375

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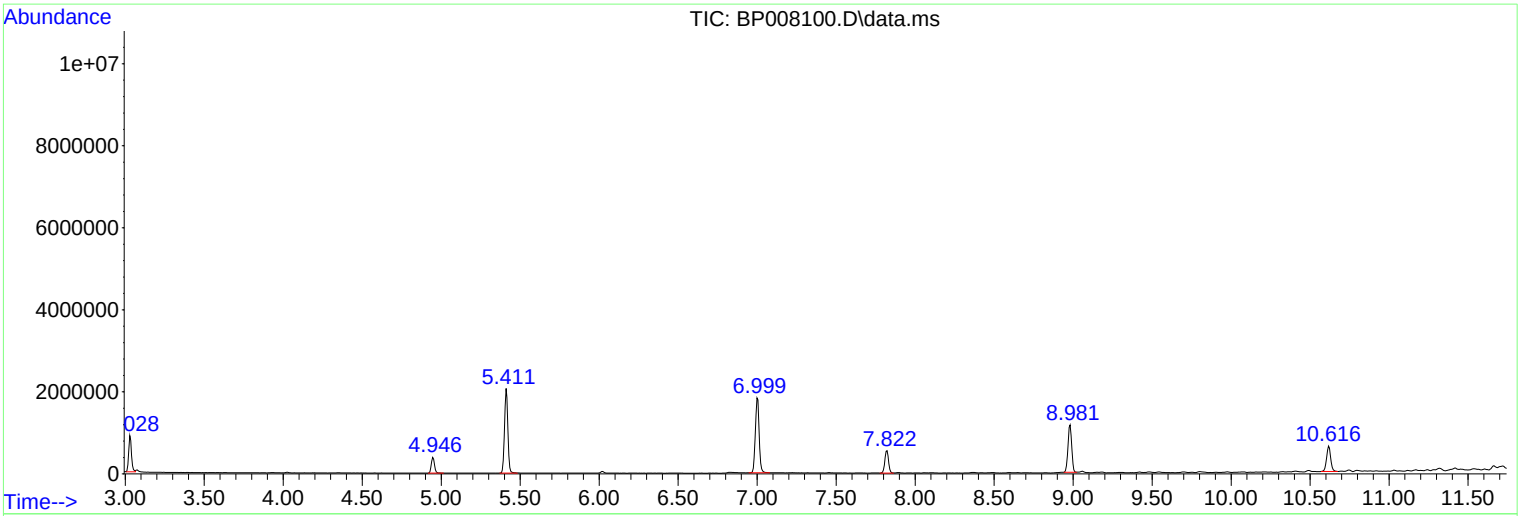
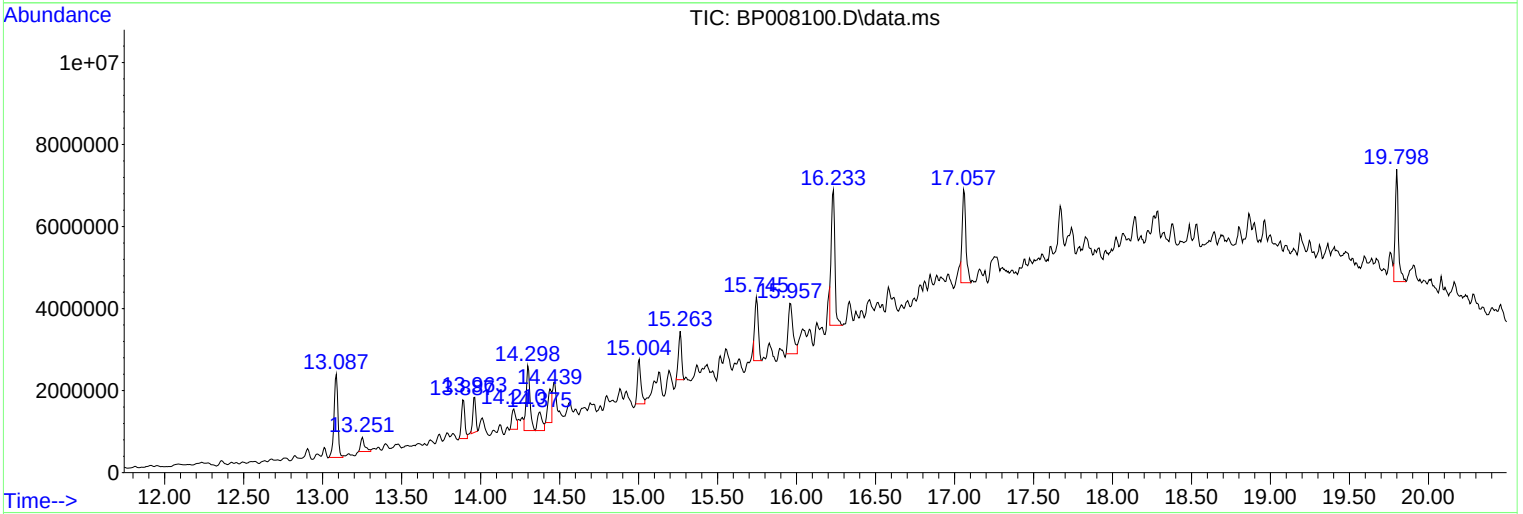
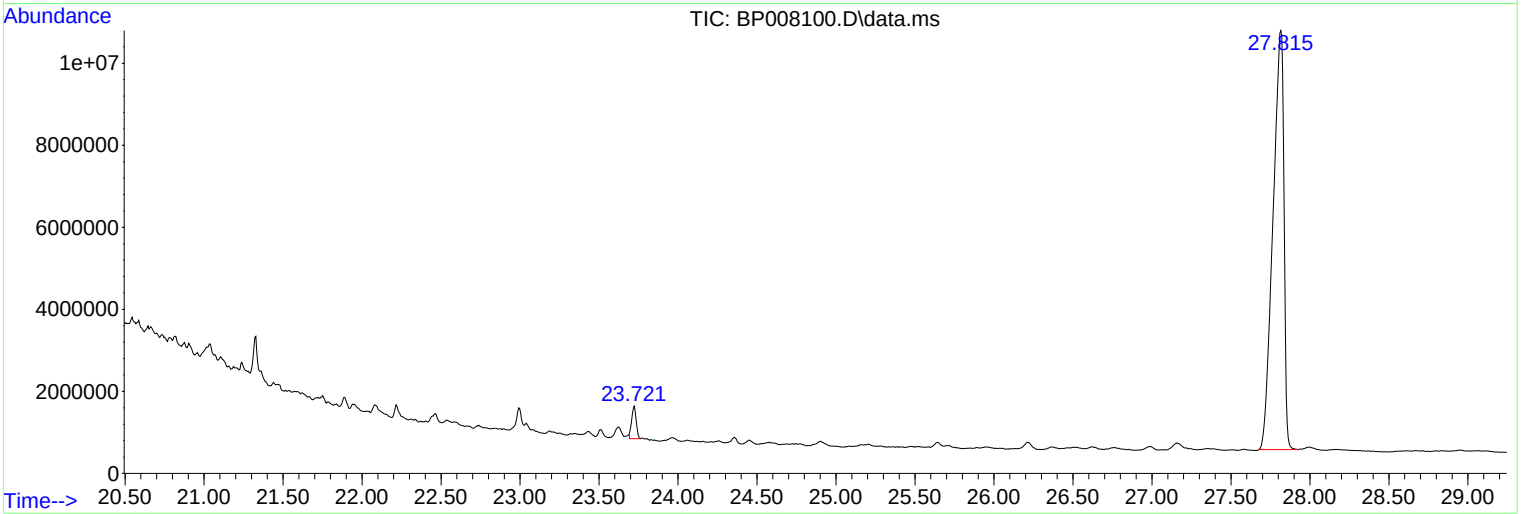
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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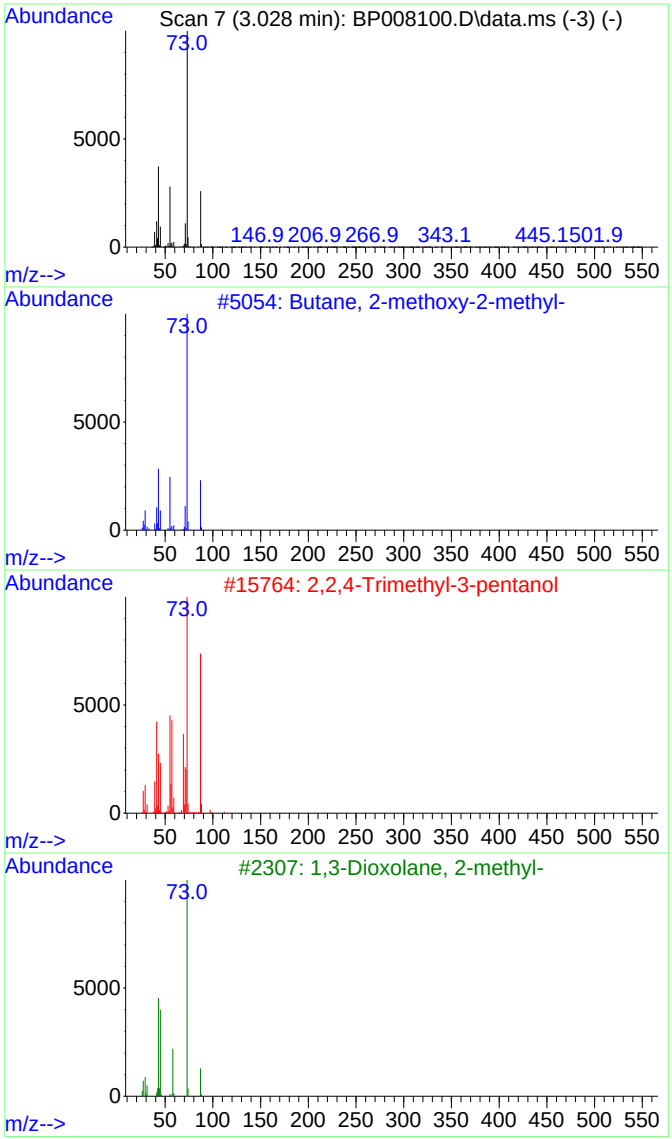
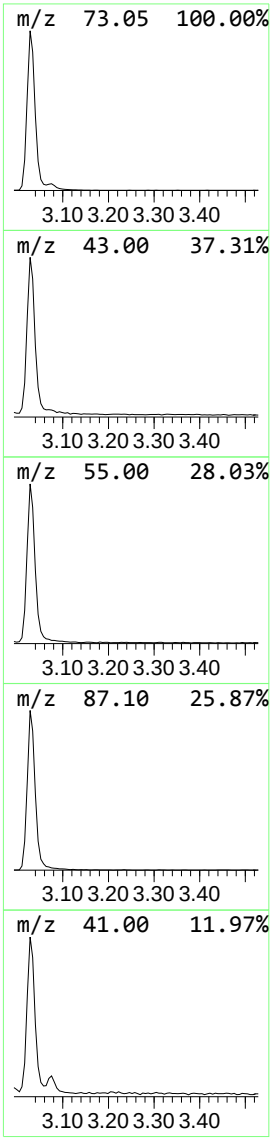
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	23.91 ng	1069960	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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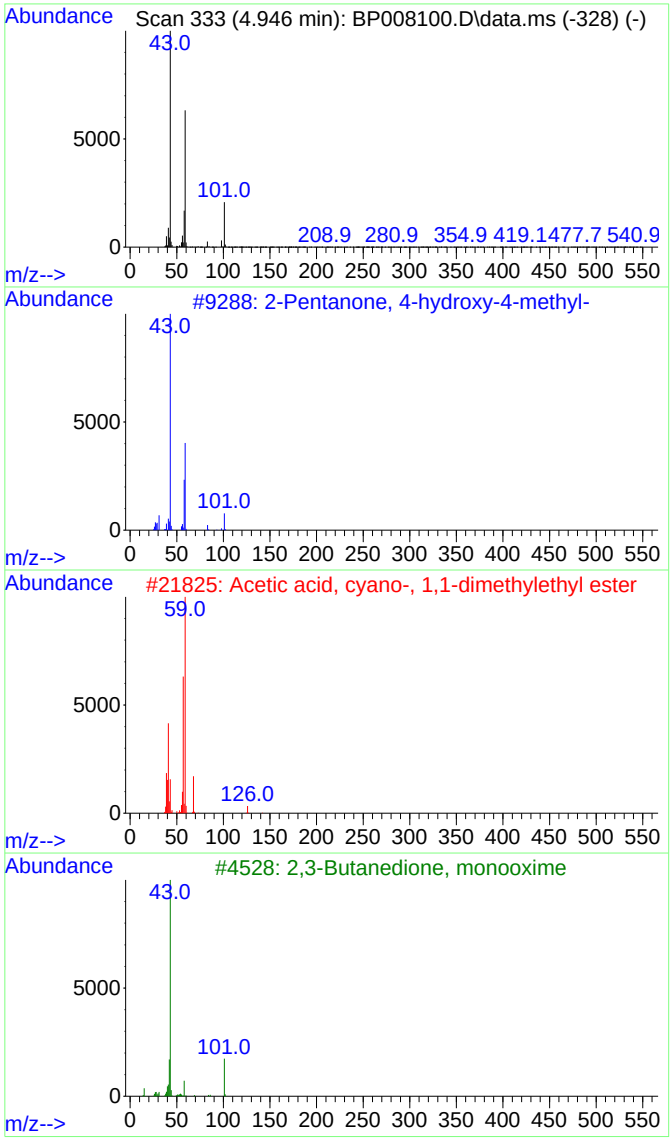
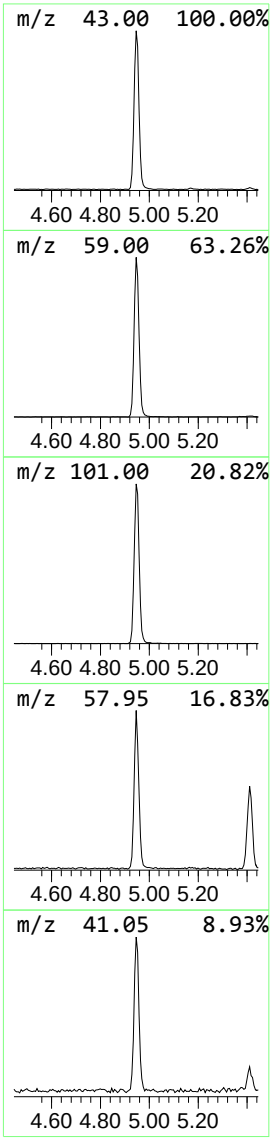
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	12.01 ng	537464	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Hexanamide	115	C6H13NO	000628-02-4	9





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BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
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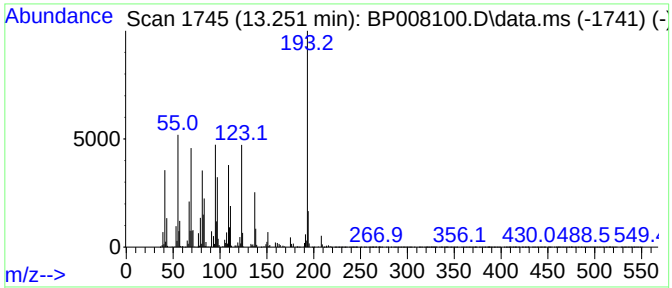
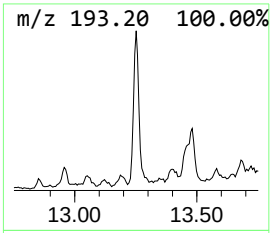
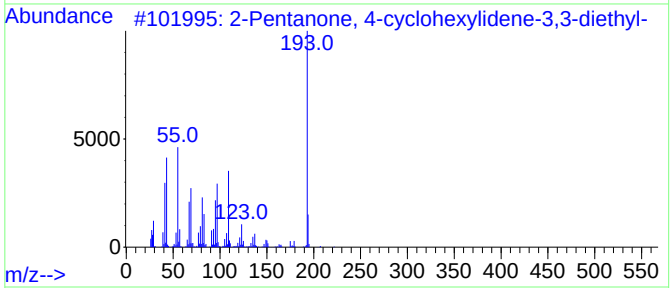
****
Peak Number 3 2-Pentanone, 4-cyclohexylid... Concentration Rank 13

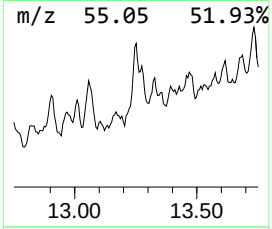
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.251	8.87 ng	633660	Acenaphthene-d10	14.463

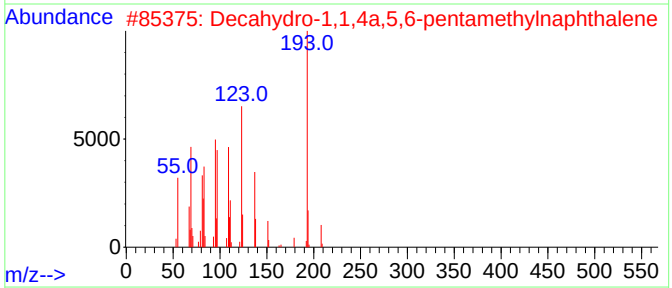
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	52
2	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	47
3	2-Amino-4-benzylthiomethyl-6-pip...	315	C16H21N5S	022362-19-2	27
4	6-Methylphenanthridine	193	C14H11N	003955-65-5	25
5	Benzo[f]quinoline, 2-methyl-	193	C14H11N	039258-30-5	22

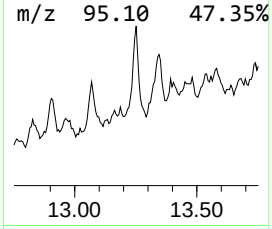


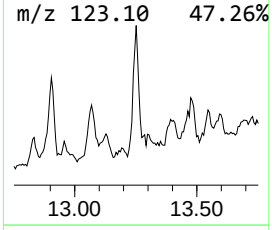


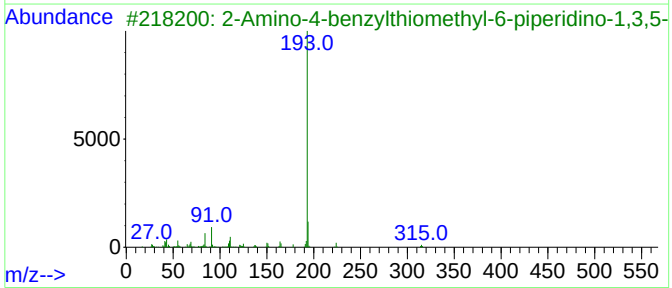


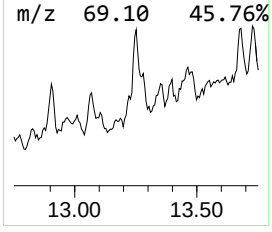












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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

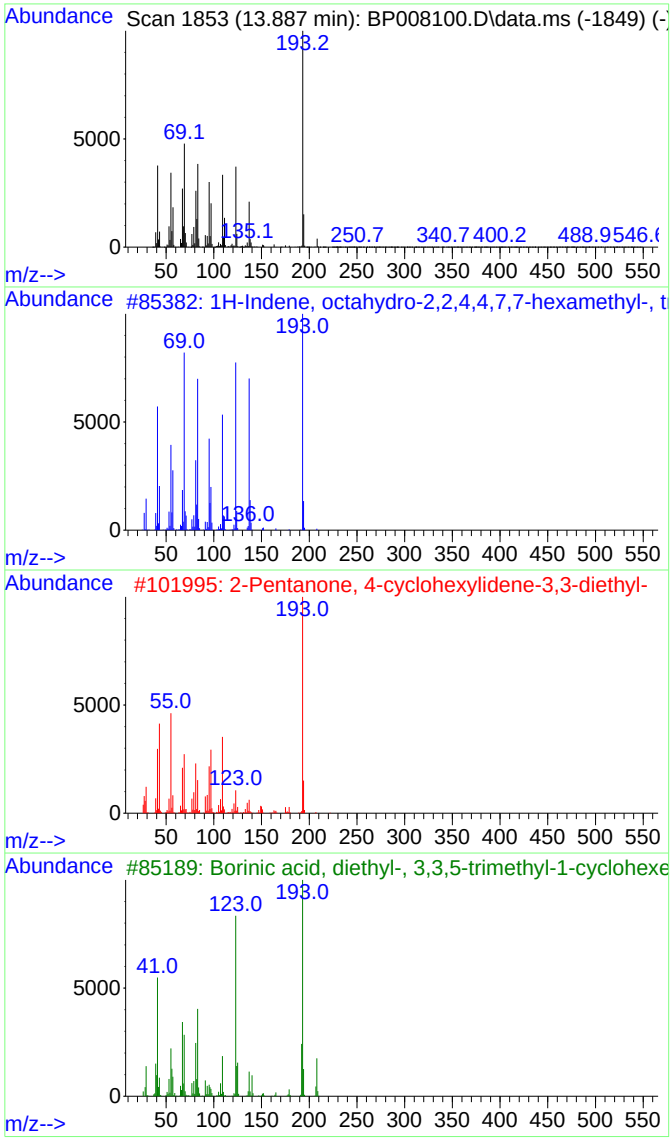
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

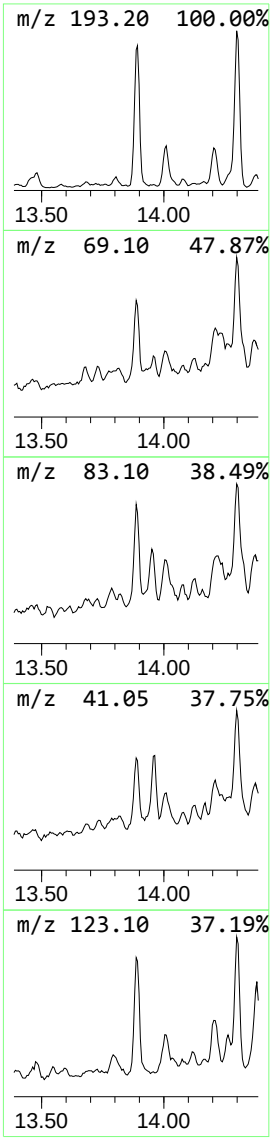
****

Peak Number 4 unknown13.887 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.887	19.87 ng	1419170	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	45
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	40
3	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	40
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
5	1-Methyl-3-(trifluoromethyl)-1H-...	193	C7H10F3N3	1000511-73-1	38





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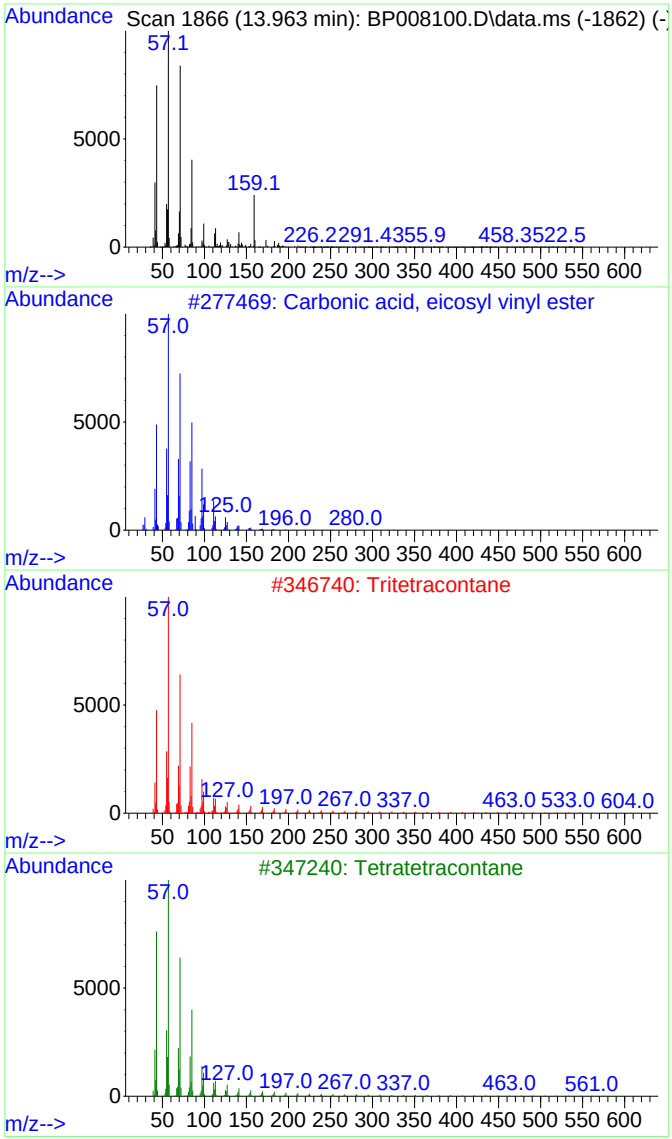
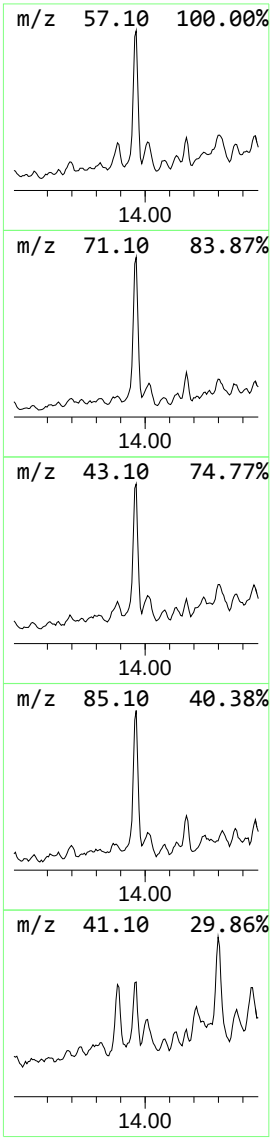
****
Peak Number 5 Carbonic acid, eicosyl viny... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	15.44 ng	1102510	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	80
2	Tritetracontane	605	C43H88	007098-21-7	72
3	Tetratetracontane	619	C44H90	007098-22-8	64
4	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	58
5	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	53





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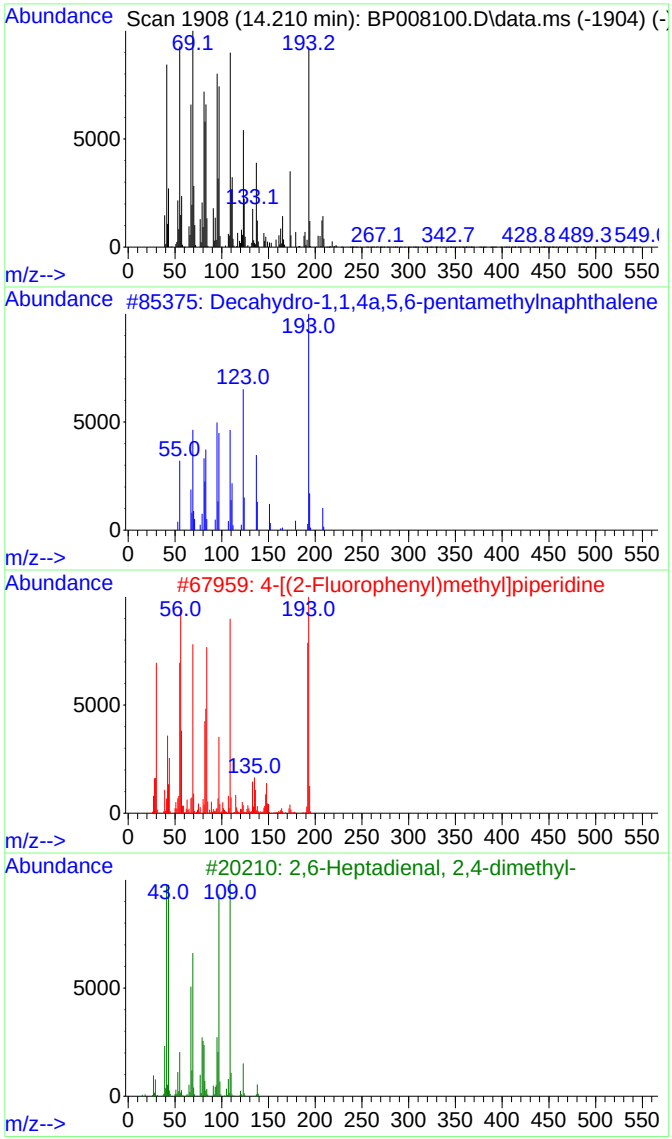
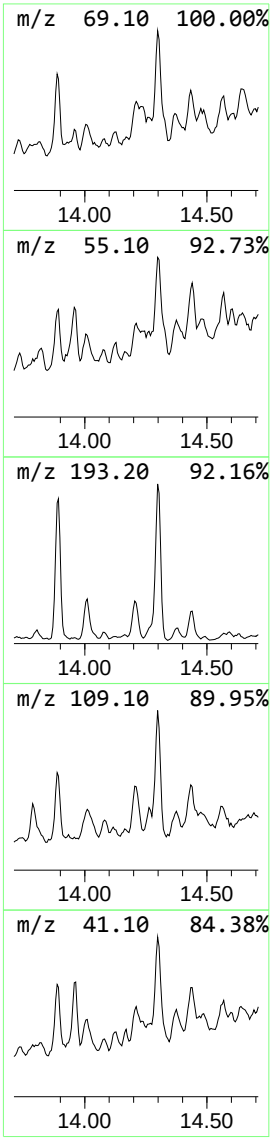
****
Peak Number 6 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.210	12.73 ng	909171	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...	208	C15H28	080655-44-3	70
2	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	50
3	2,6-Heptadienal, 2,4-dimethyl-	138	C9H14O	085136-08-9	50
4	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	30
5	Cyclopropane, 1,1-dimethyl-2-(2-...	124	C9H16	069147-03-1	20





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TIC Library : C:\Database\NIST20.L
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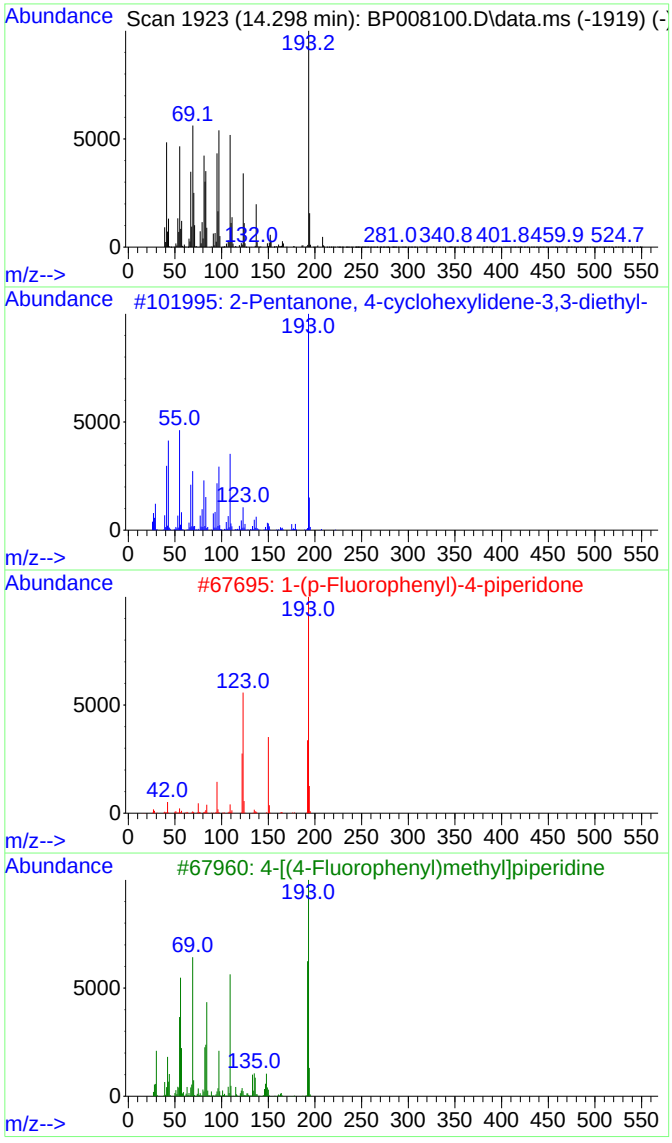
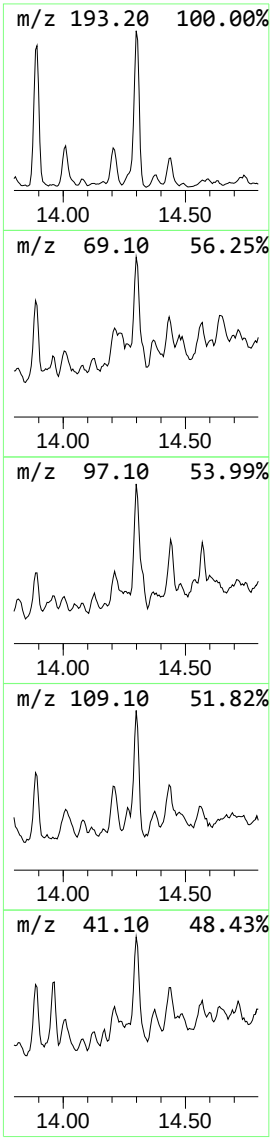
Peak Number 7 unknown14.298 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.298	36.68 ng	2619060	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	45
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	38
3	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	37
4	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	36
5	2-Amino-4-ethylthiomethyl-6-pipe...	253	C11H19N5S	022362-22-7	27





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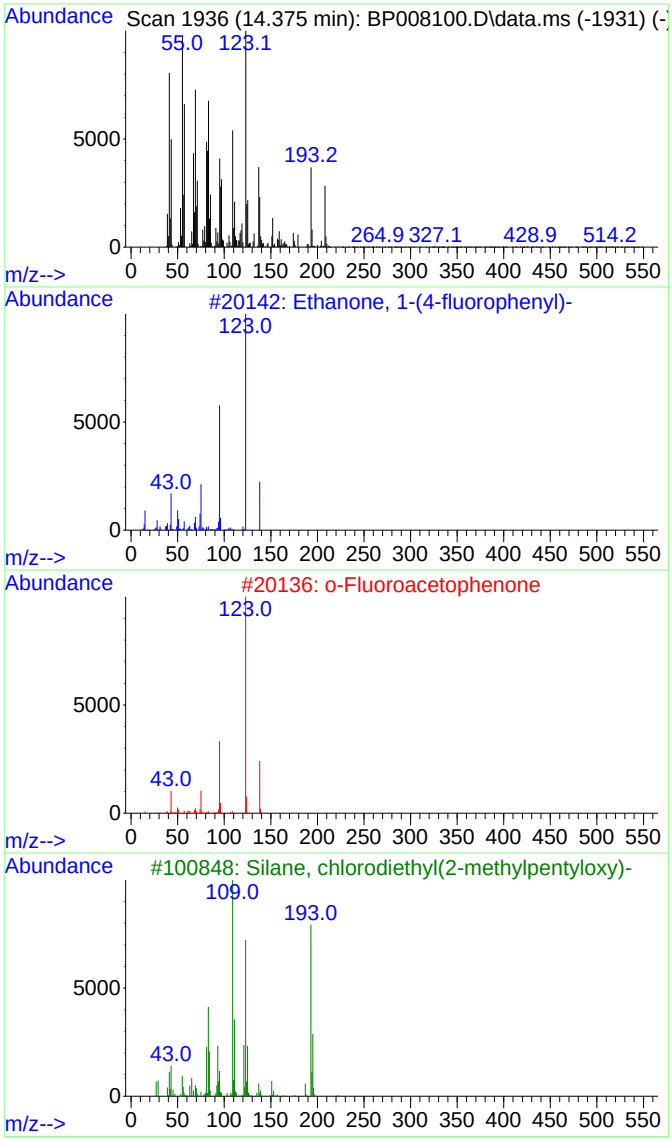
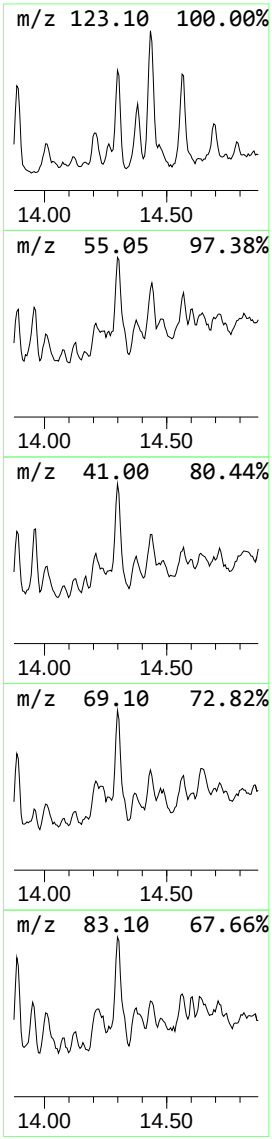
Peak Number 8 unknown14.375 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.375	13.38 ng	955516	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	000403-42-9	38
2	o-Fluoroacetophenone	138	C8H7FO	000445-27-2	35
3	Silane, chlorodiethyl(2-methylpe...	222	C10H23ClOSi	1000363-12-7	30
4	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	30
5	Diethyl 1-(carbethoxy)ethylphosp...	238	C9H19O5P	1000306-25-7	30





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Data File : BP008100.D
Acq On : 23 Nov 2021 17:21
Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

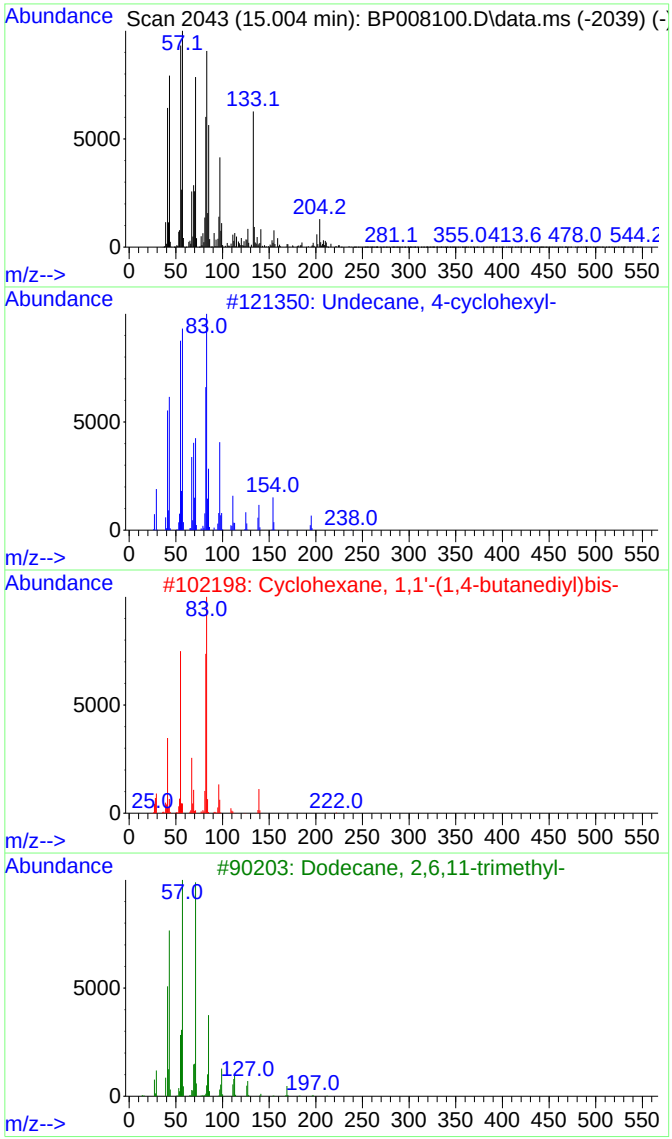
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

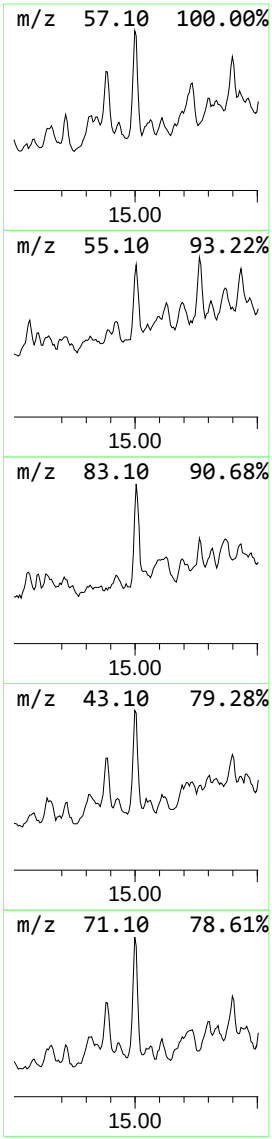
****

Peak Number 9 unknown15.004 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.004	23.46 ng	1675210	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 4-cyclohexyl-	238	C17H34	013151-79-6	49
2	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	38
3	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	35
4	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	30
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	30





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Acq On : 23 Nov 2021 17:21
Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

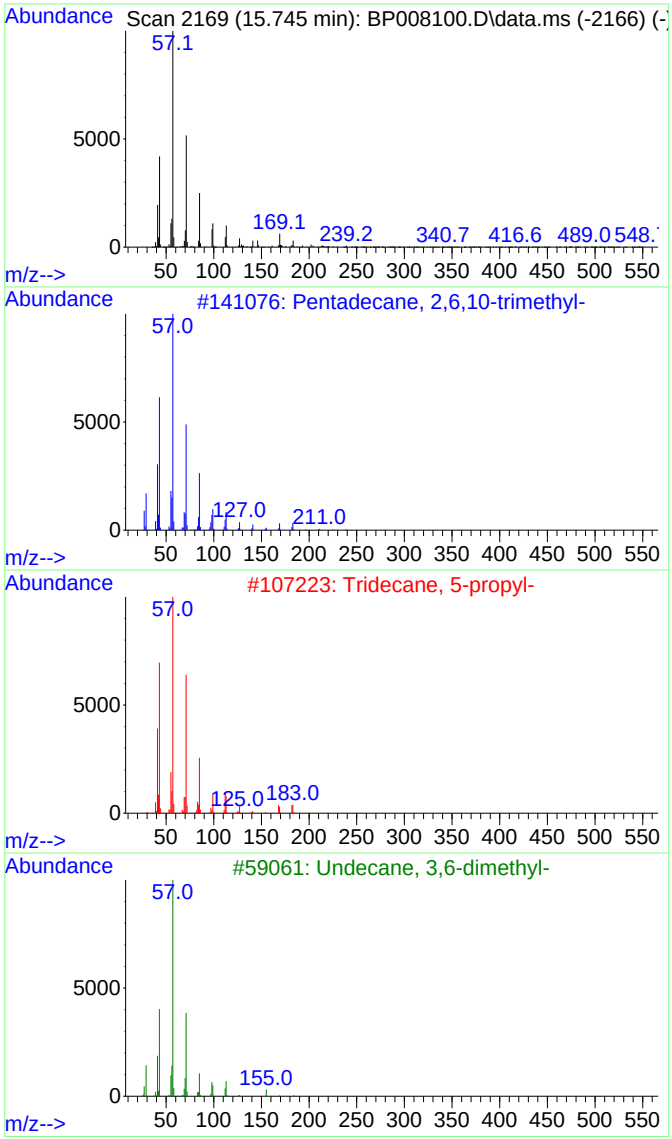
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

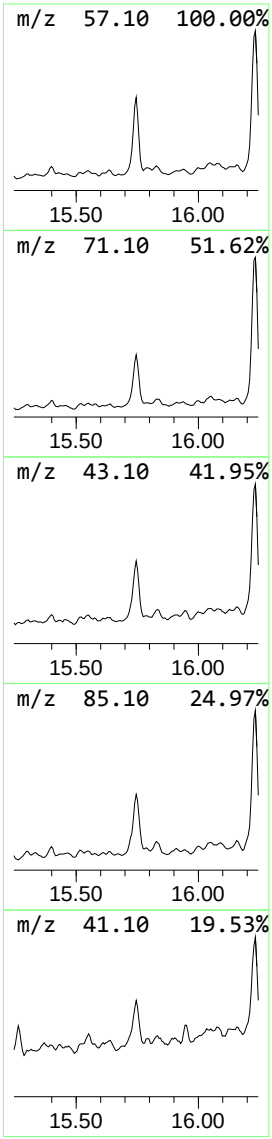
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentadecane, 2,6,10-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.745	32.55 ng	2324640	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	91
2	Tridecane, 5-propyl-	226	C16H34	055045-11-9	87
3	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	76
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	72
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72





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Acq On : 23 Nov 2021 17:21
Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
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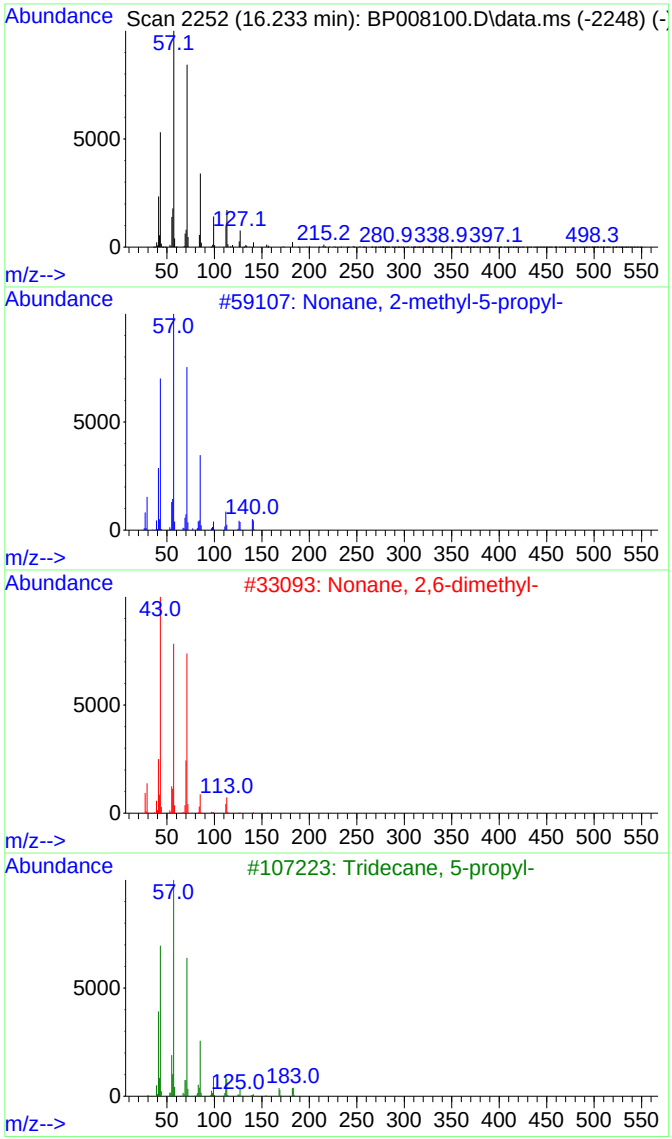
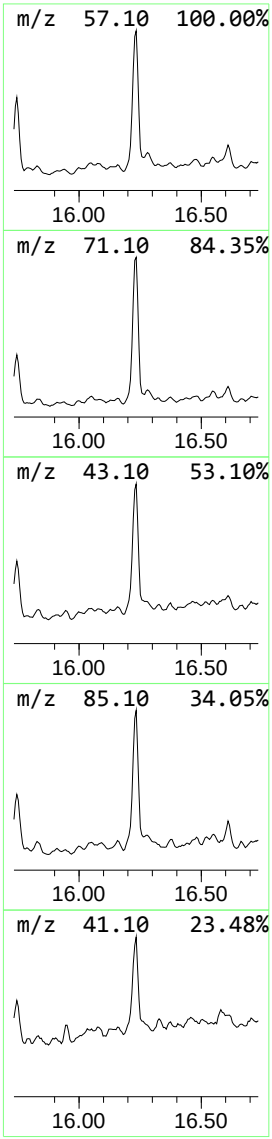
Peak Number 11 Nonane, 2-methyl-5-propyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.233	28.65 ng	5209690	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 2-methyl-5-propyl-	184	C13H28	031081-17-1	78
2	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	72
3	Tridecane, 5-propyl-	226	C16H34	055045-11-9	72
4	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	64
5	Hexadecane	226	C16H34	000544-76-3	64





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Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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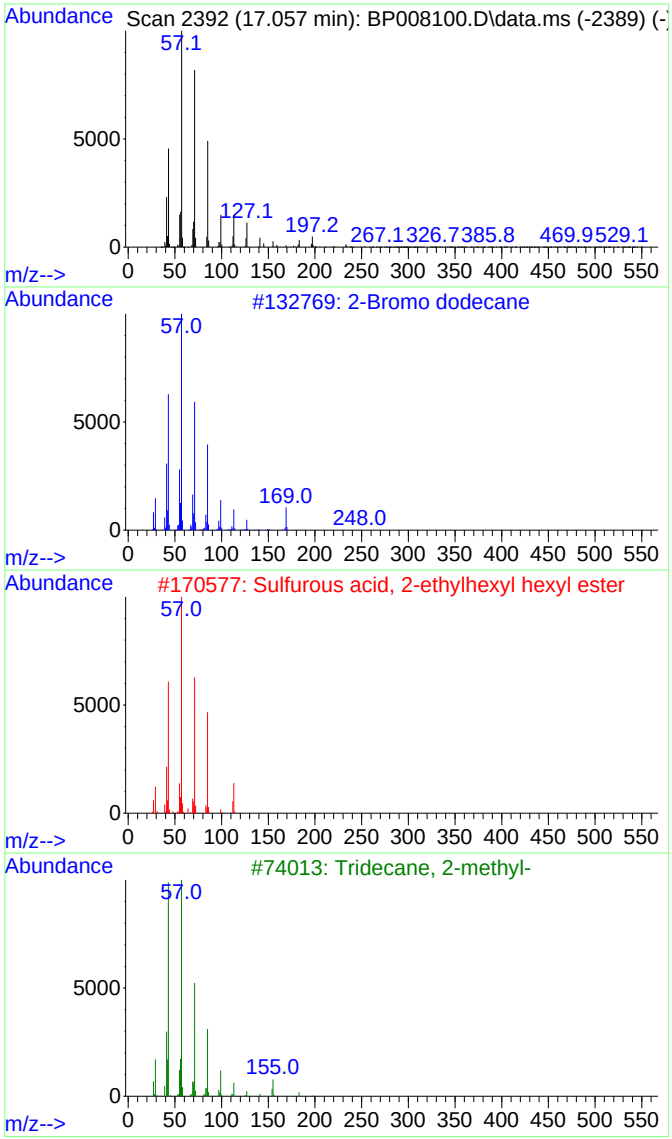
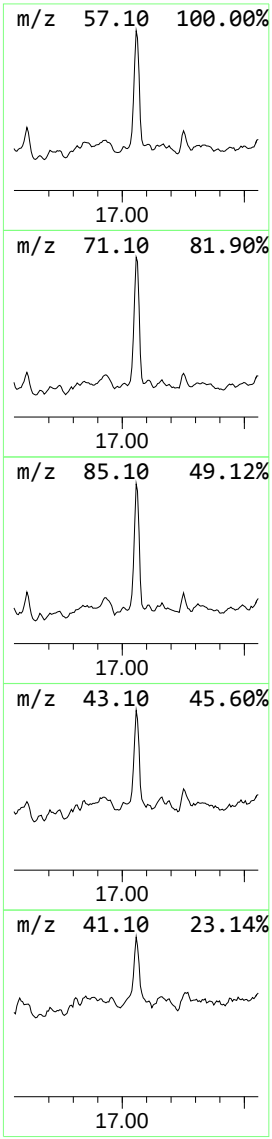
Peak Number 12 2-Bromo dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.057	20.00 ng	3636250	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane	248	C12H25Br	013187-99-0	78
2	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	60
5	Decane, 5-ethyl-5-methyl-	184	C13H28	017312-74-2	59





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Data File : BP008100.D
Acq On : 23 Nov 2021 17:21
Operator : CG/JU
Sample : M4811-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20071

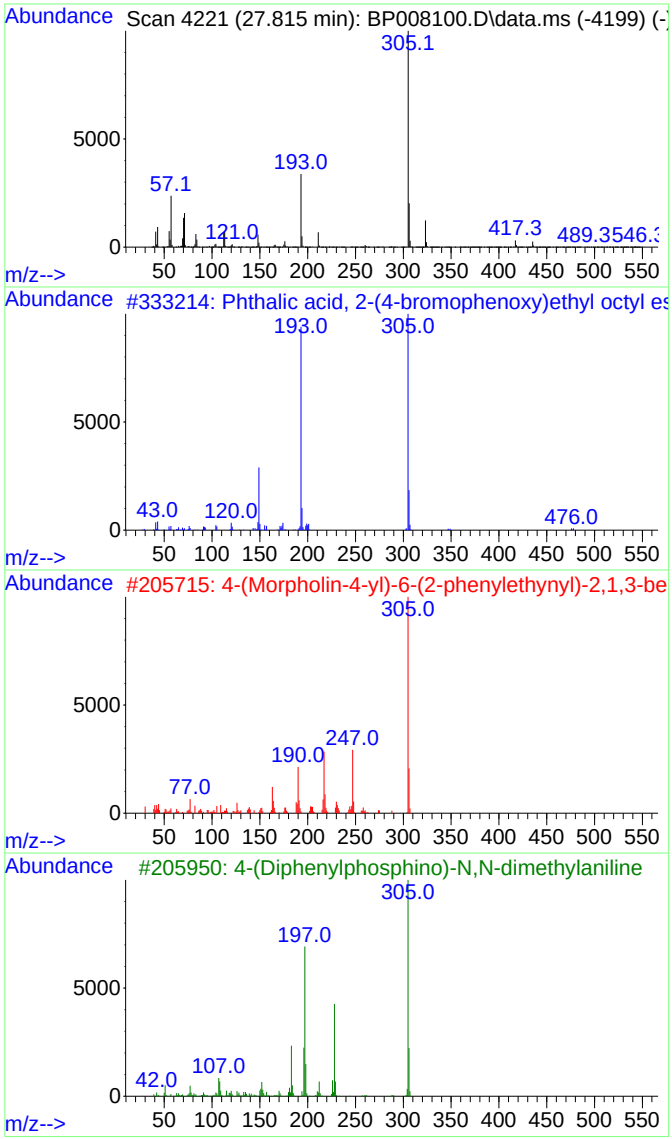
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

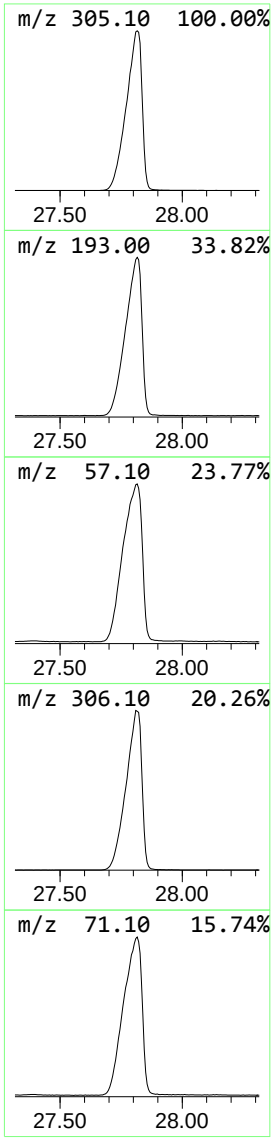
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Phthalic acid, 2-(4-bromoph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.815	631.35 ng	49082200	Perylene-d12	23.721

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 2-(4-bromophenoxy...	476	C24H29BrO5	1010382-89-7	72
2	4-(Morpholin-4-yl)-6-(2-phenylet...	305	C18H15N3O2	1000387-57-0	40
3	4-(Diphenylphosphino)-N,N-dimeth...	305	C20H20NP	000739-58-2	36
4	2,3-Dihydroxybutanedihydrazide, ...	610	C22H58N4O4Si6	1000511-48-0	36
5	Furo[2,3-H]coumarine, 6-methyl-1...	305	C19H15NO3	1000270-15-3	33





Tentatively Identified Compound (LSC) summary

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Data File : BP008100.D
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BNA_P
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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
Butane, 2-metho...	3.028	23.9	ng	1069960	1	7.822	895109	20.0
2-Pentanone, 4-...	4.946	12.0	ng	537464	1	7.822	895109	20.0
2-Pentanone, 4-...	13.251	8.9	ng	633660	3	14.463	1428190	20.0
unknown13.887	13.887	19.9	ng	1419170	3	14.463	1428190	20.0
Carbonic acid, ...	13.963	15.4	ng	1102510	3	14.463	1428190	20.0
Decahydro-1,1,4...	14.210	12.7	ng	909171	3	14.463	1428190	20.0
unknown14.298	14.298	36.7	ng	2619060	3	14.463	1428190	20.0
unknown14.375	14.375	13.4	ng	955516	3	14.463	1428190	20.0
unknown15.004	15.004	23.5	ng	1675210	3	14.463	1428190	20.0
Pentadecane, 2,...	15.745	32.5	ng	2324640	3	14.463	1428190	20.0
Nonane, 2-methy...	16.233	28.6	ng	5209690	4	17.233	3636250	20.0
2-Bromo dodecane	17.057	20.0	ng	3636250	4	17.233	3636250	20.0
Phthalic acid, ...	27.815	631.4	ng	49082200	6	23.721	1554830	20.0