

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
 Data File : BF093770.D
 Acq On : 20 Mar 2017 18:02
 Operator : SJ/MA
 Sample : I2271-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BHP-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.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	2.115	18	20	23	rBV	110025	128948	2.36%	0.265%
2	5.018	271	274	280	rBV	502671	712783	13.04%	1.468%
3	5.441	307	311	313	rBV	4005753	5082600	93.01%	10.464%
4	6.470	397	401	403	rBV	4215456	5464459	100.00%	11.250%
5	6.607	409	413	415	rBV	4048989	5219136	95.51%	10.745%
6	6.836	430	433	435	rBV	1836416	1581119	28.93%	3.255%
7	6.996	444	447	449	rVB	3829266	3921891	71.77%	8.075%
8	7.396	479	482	484	rBV	3132301	3150041	57.65%	6.485%
9	7.647	498	504	506	rBV3	32649	71725	1.31%	0.148%
10	8.116	543	545	548	rBV	2032416	2022979	37.02%	4.165%
11	8.562	581	584	586	rBV	57937	74764	1.37%	0.154%
12	9.202	637	640	642	rVB	4815224	5327930	97.50%	10.969%
13	9.282	645	647	650	rBV2	47840	82495	1.51%	0.170%
14	9.533	666	669	672	rBV3	37695	91584	1.68%	0.189%
15	9.590	672	674	675	rVV	517126	471672	8.63%	0.971%
16	9.613	675	676	677	rVB	85910	60604	1.11%	0.125%
17	9.865	696	698	701	rBV	1662054	2224056	40.70%	4.579%
18	10.070	712	716	718	rBV5	29111	71990	1.32%	0.148%
19	10.150	721	723	725	rBV2	52881	90535	1.66%	0.186%
20	10.322	736	738	739	rVV	58627	81886	1.50%	0.169%
21	10.539	754	757	760	rBV	83562	107864	1.97%	0.222%
22	10.653	764	767	770	rVB	2715100	2671914	48.90%	5.501%
23	10.802	777	780	782	rBV	169993	275661	5.04%	0.568%
24	11.236	816	818	819	rBV2	106082	105080	1.92%	0.216%
25	11.271	819	821	823	rVB	53933	70135	1.28%	0.144%
26	11.351	825	828	830	rBV	1779633	1991123	36.44%	4.099%
27	11.659	853	855	857	rBV	58745	54996	1.01%	0.113%
28	11.888	873	875	876	rBV2	57444	56450	1.03%	0.116%
29	12.551	932	933	935	rBV	60703	64736	1.18%	0.133%
30	12.608	935	938	940	rVV3	27377	55919	1.02%	0.115%
31	12.779	950	953	954	rBV	50236	61578	1.13%	0.127%
32	12.928	964	966	969	rBV	3150820	3438765	62.93%	7.080%
33	13.831	1043	1045	1051	rVB	173939	237567	4.35%	0.489%
34	13.968	1055	1057	1060	rBV	1446534	1383333	25.32%	2.848%

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35	14.471	1098	1101	1103	rBV	95909	143431	2.62%	0.295%
36	14.974	1143	1145	1146	rBV	56487	72169	1.32%	0.149%
37	15.374	1177	1180	1183	rBV	870754	1166227	21.34%	2.401%
38	15.900	1223	1226	1230	rVB5	37442	95069	1.74%	0.196%
39	16.060	1238	1240	1247	rVB2	64969	146664	2.68%	0.302%
40	16.471	1273	1276	1280	rVB	60673	121467	2.22%	0.250%
41	17.488	1362	1365	1367	rBV3	23277	54913	1.00%	0.113%
42	18.883	1483	1487	1493	rBV7	29045	103152	1.89%	0.212%
43	19.031	1496	1500	1506	rVB7	25935	84121	1.54%	0.173%
44	19.237	1516	1518	1525	rVB8	20881	75433	1.38%	0.155%

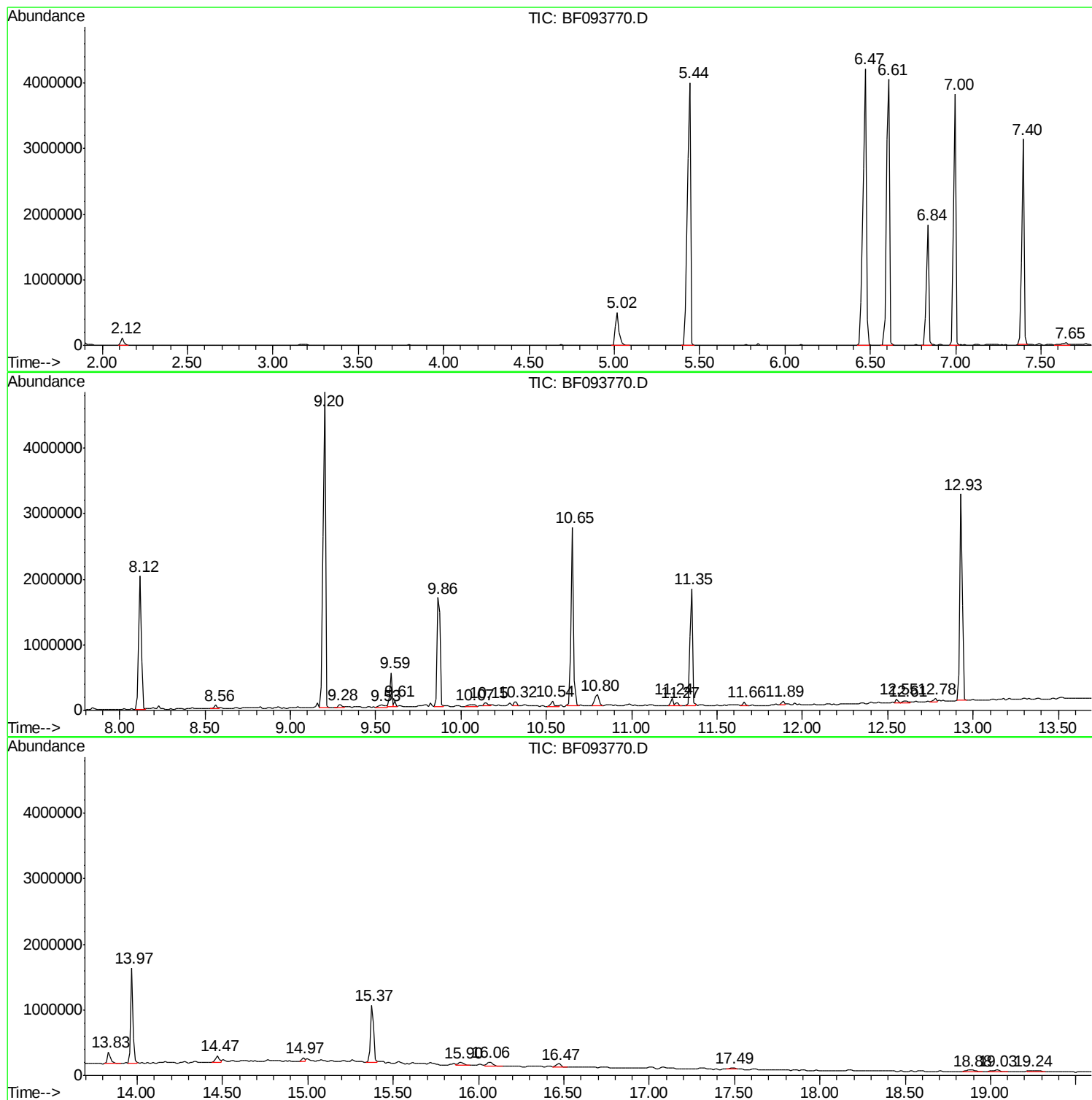
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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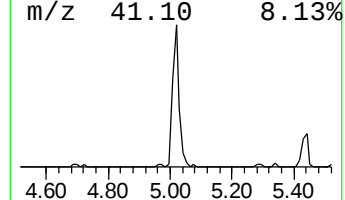
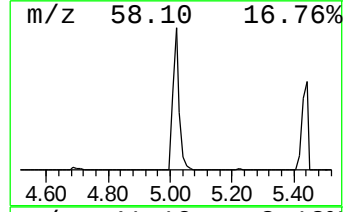
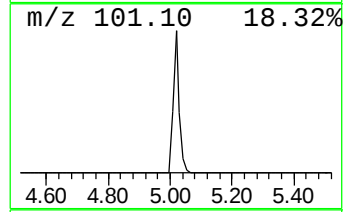
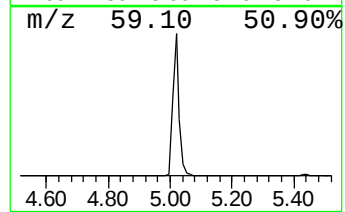
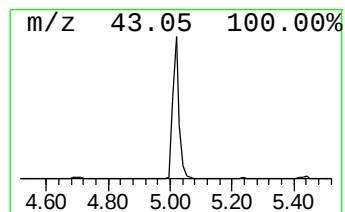
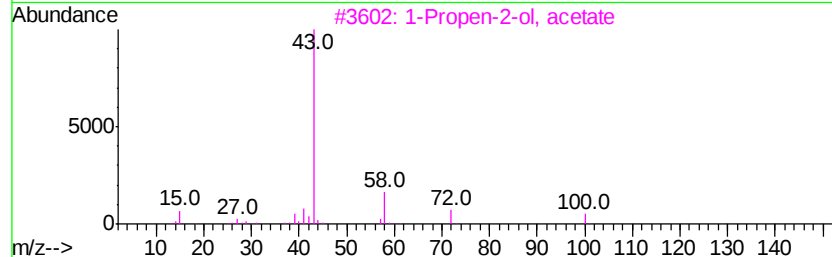
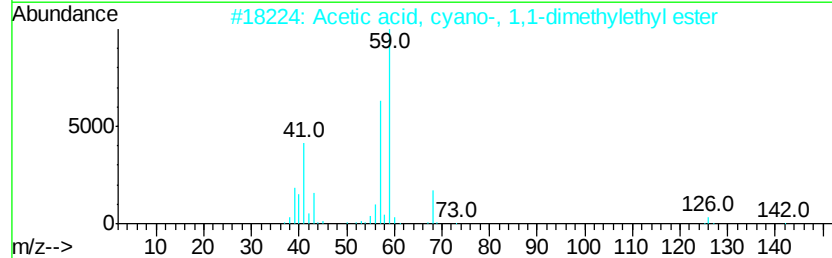
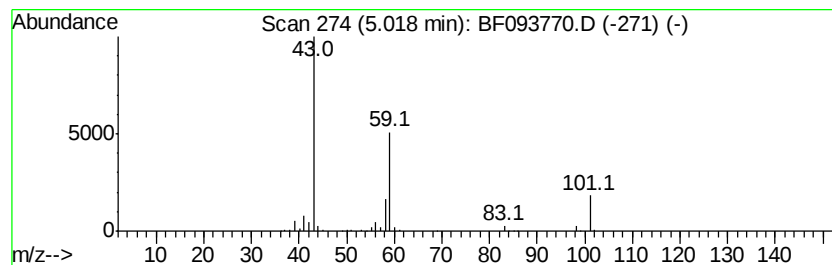
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	9.02 ng	712783	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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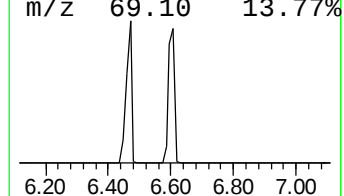
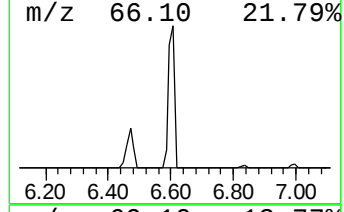
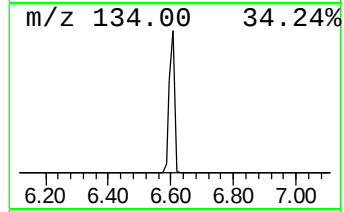
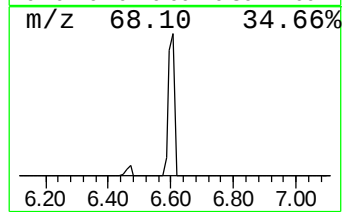
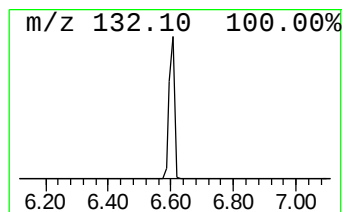
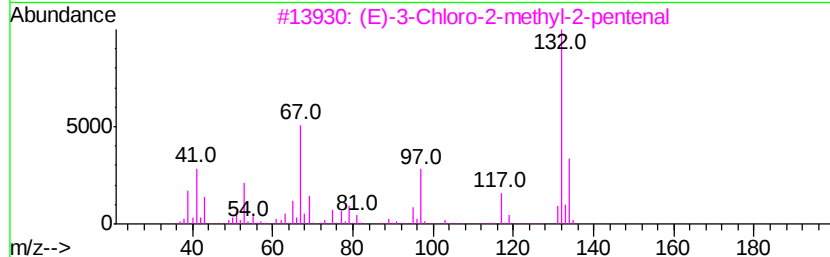
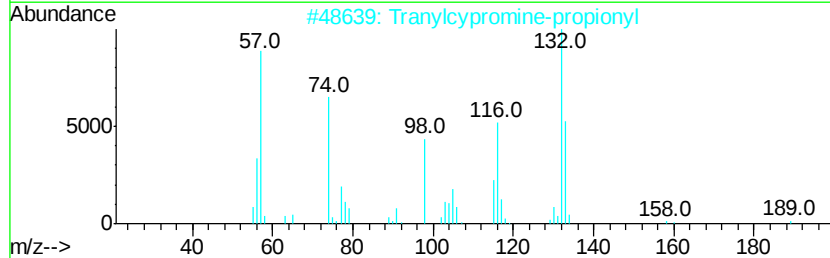
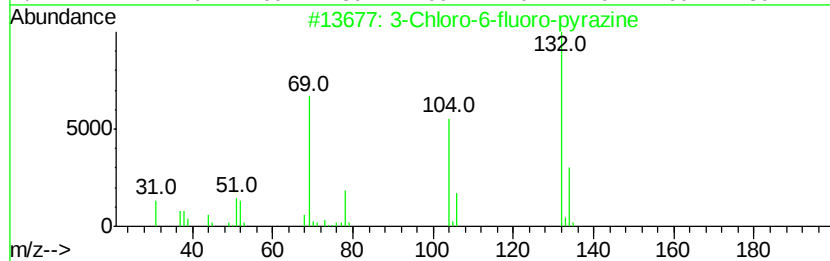
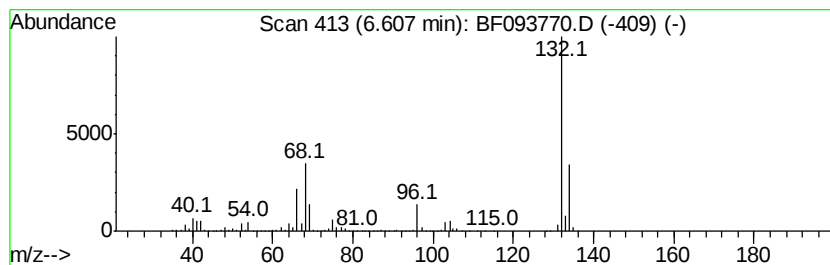
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Peak Number 2 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	66.02 ng	5219140	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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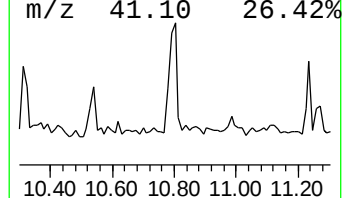
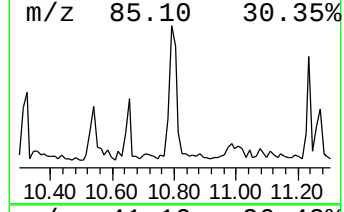
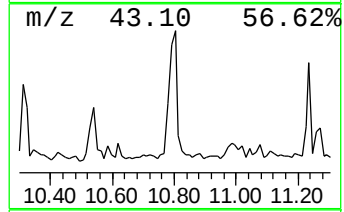
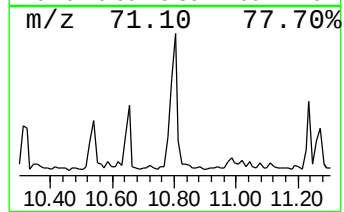
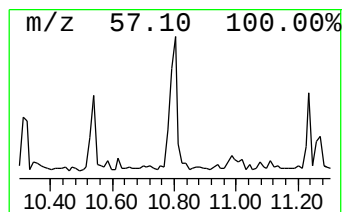
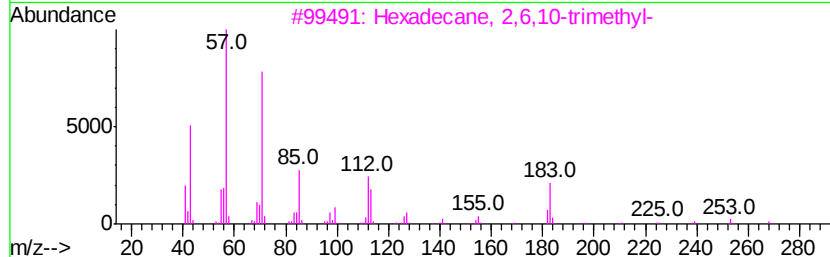
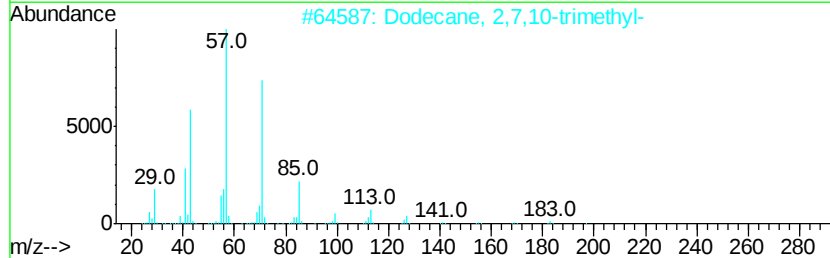
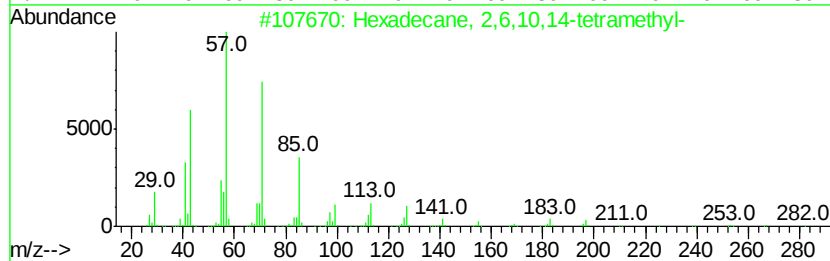
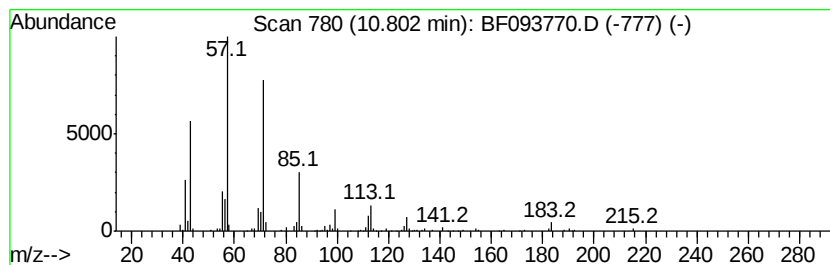
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Peak Number 4 Hexadecane, 2,6,10,14-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	2.77 ng	275661	Phenanthrene-d10	11.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
3		Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	83
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	80
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78



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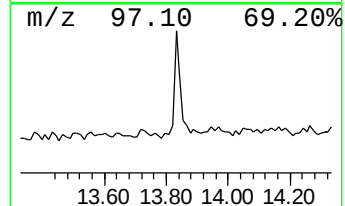
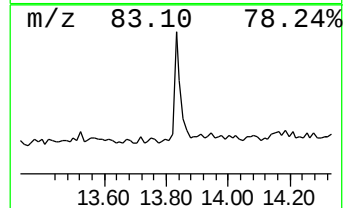
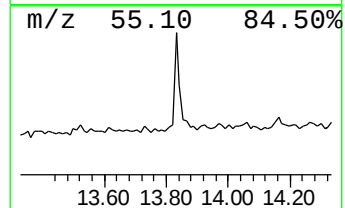
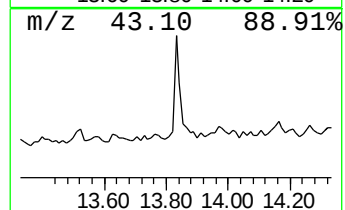
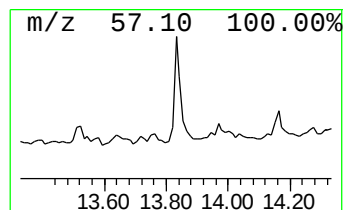
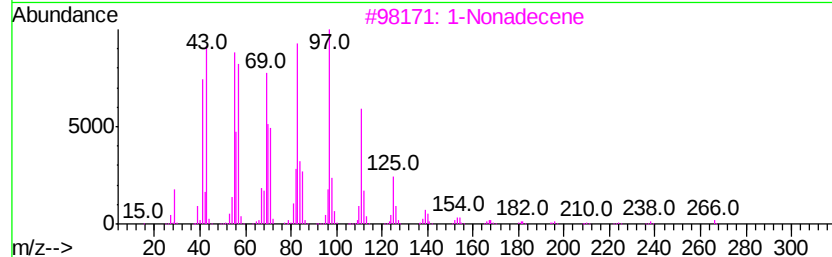
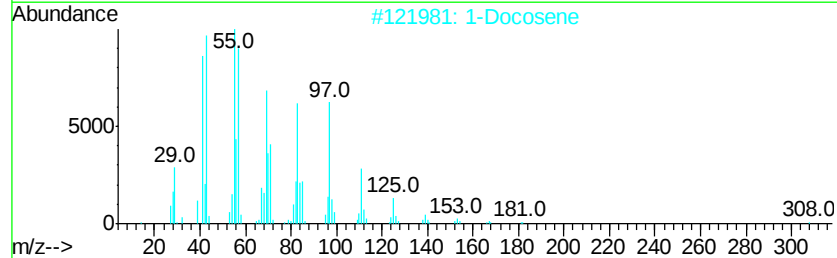
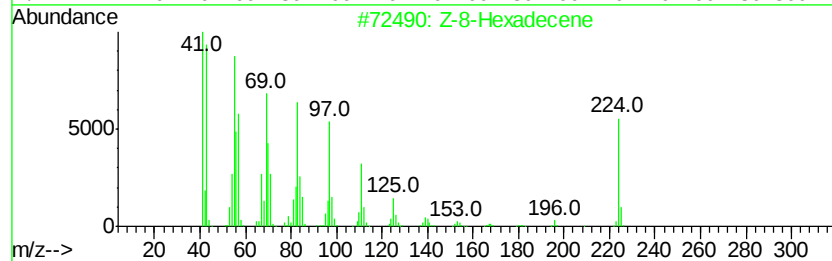
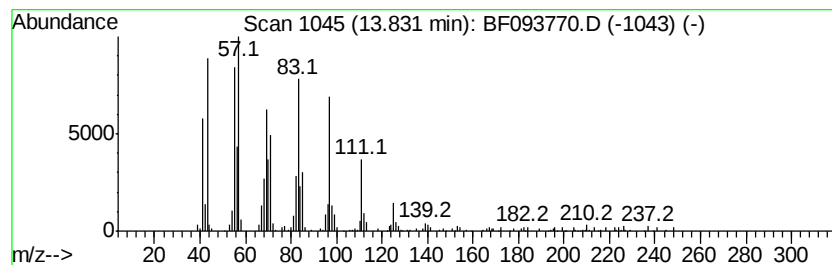
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Peak Number 5 Z-8-Hexadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	3.43 ng	237567	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Z-8-Hexadecene	224	C16H32	1000130-87-5	93
2		1-Docosene	308	C22H44	001599-67-3	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		1-Heptadecanol	256	C17H36O	001454-85-9	90
5		Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	87



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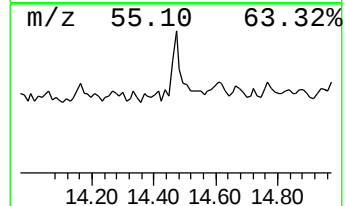
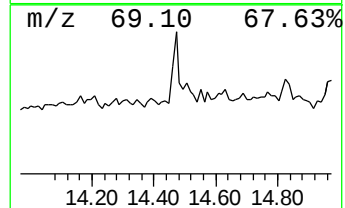
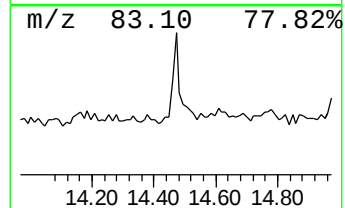
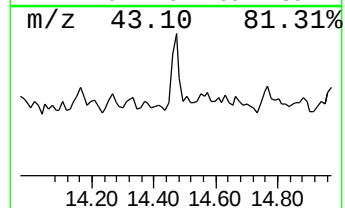
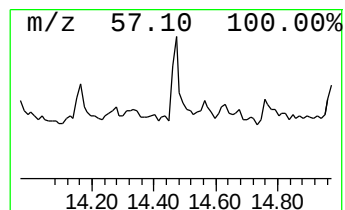
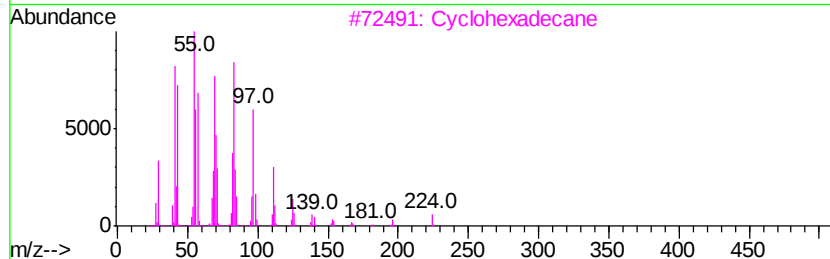
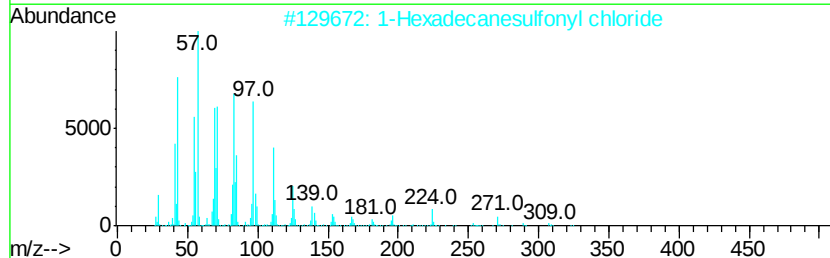
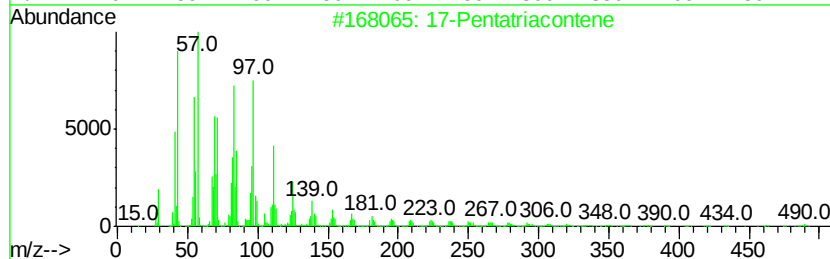
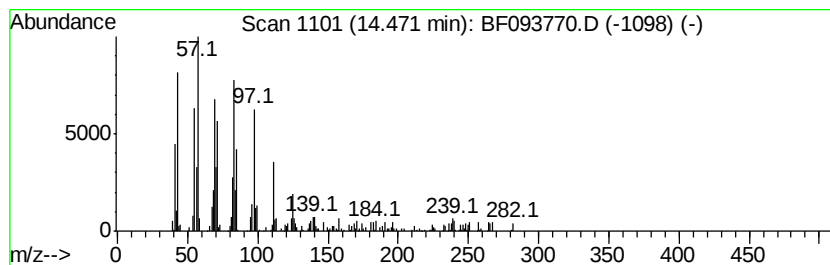
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Peak Number 6 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.07 ng	143431	Chrysene-d12	13.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	90
2		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3		Cyclohexadecane	224	C16H32	000295-65-8	83
4		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	83
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093770.D
Acq On : 20 Mar 2017 18:02
Operator : SJ/MA
Sample : I2271-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BHP-1

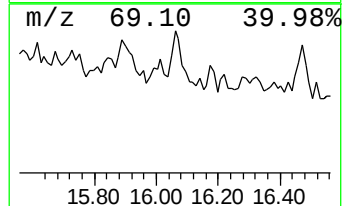
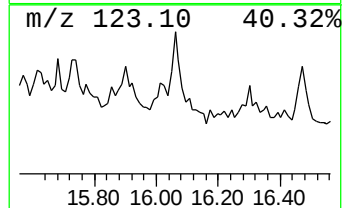
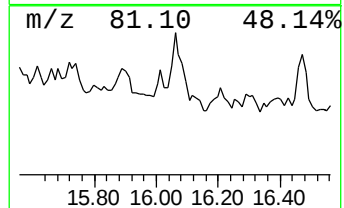
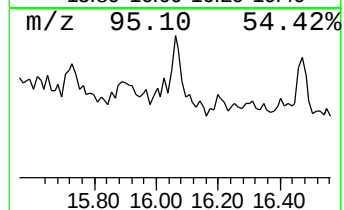
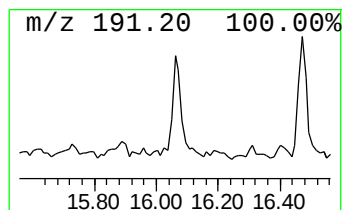
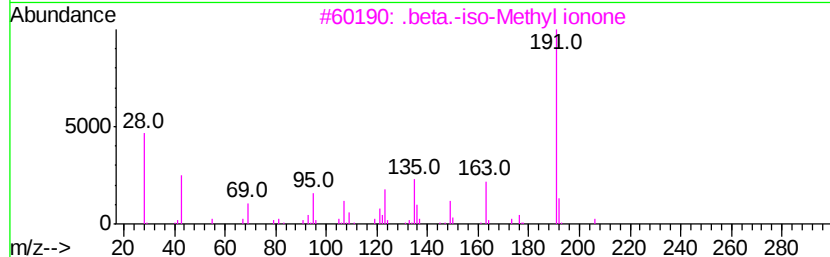
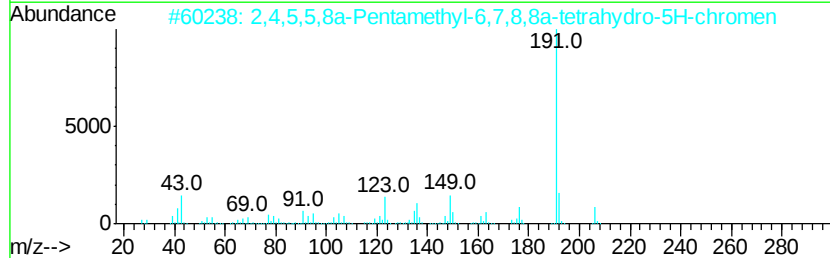
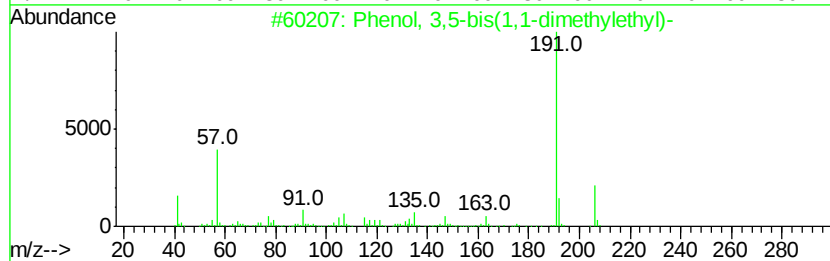
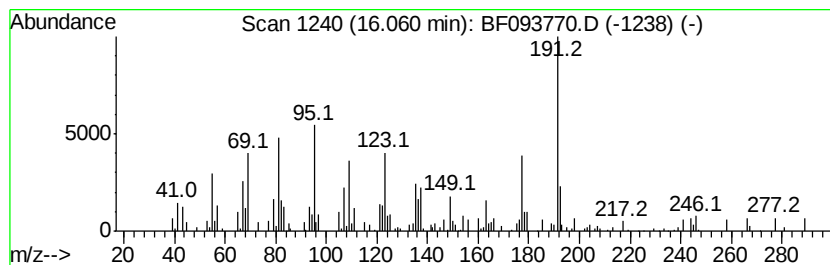
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.06 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.06	2.52 ng	146664	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	30
2		2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	27
3		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	25
4		Isoquinoline, 1,2,3,4-tetrahydro...	283	C18H21NO2	036646-87-4	25
5		1H-Pyrrolo[3,4-c]pyridine-1,3,(2...	191	C9H9N3O2	298688-32-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF032017\
Data File : BF093770.D
Acq On : 20 Mar 2017 18:02
Operator : SJ/MA
Sample : I2271-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BHP-1

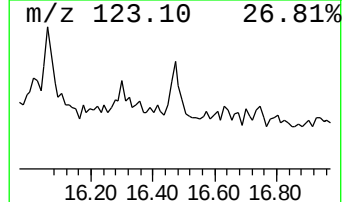
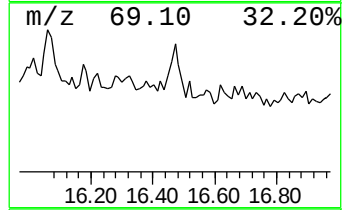
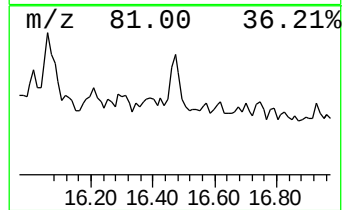
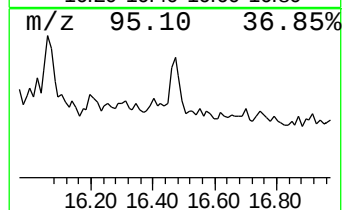
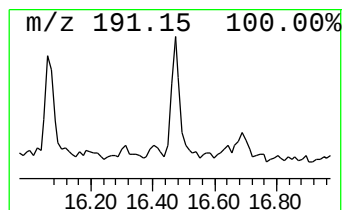
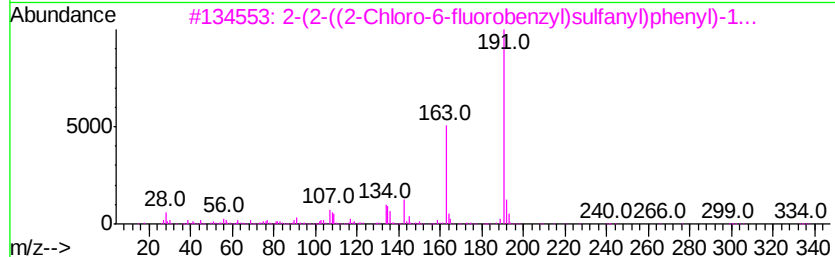
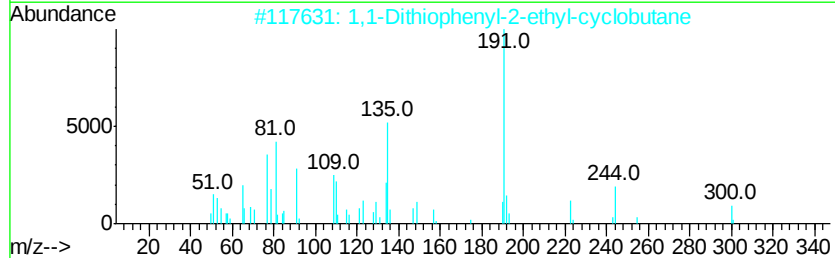
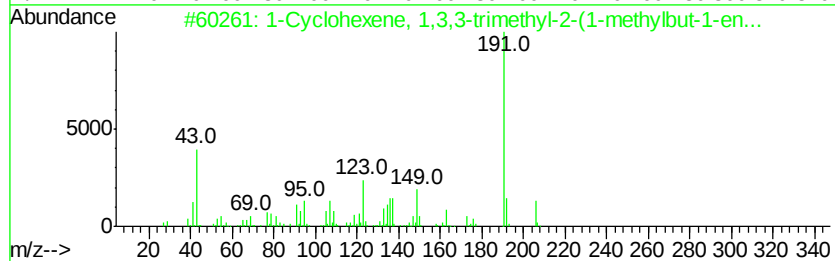
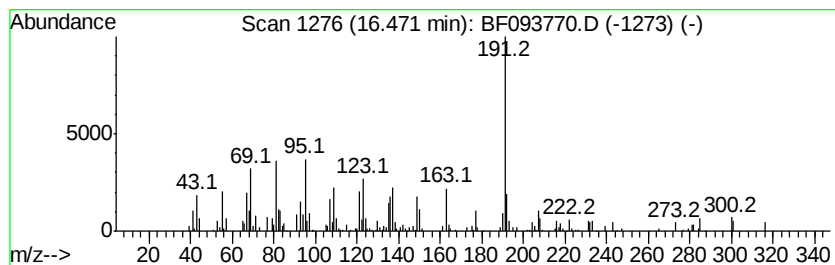
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Cyclohexene, 1,3,3-trimet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	2.08 ng	121467	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	50
2		1,1-Dithiophenyl-2-ethyl-cyclobu...	300	C18H20S2	122732-87-0	47
3		2-(2-((2-Chloro-6-fluorobenzyl)s...	334	C17H16ClFN2S	1000298-18-2	43
4		.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	40
5		2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032017\
Data File : BF093770.D
Acq On : 20 Mar 2017 18:02
Operator : SJ/MA
Sample : I2271-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BHP-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	9.0	ng	712783	1	6.84	1581120	20.0
unknown6.61	6.61	66.0	ng	5219140	1	6.84	1581120	20.0
Hexadecane, 2,6,1...	10.80	2.8	ng	275661	4	11.35	1991120	20.0
Z-8-Hexadecene	13.83	3.4	ng	237567	5	13.97	1383330	20.0
17-Pentatriacontene	14.47	2.1	ng	143431	5	13.97	1383330	20.0
unknown16.06	16.06	2.5	ng	146664	6	15.37	1166230	20.0
1-Cyclohexene, 1,...	16.47	2.1	ng	121467	6	15.37	1166230	20.0