

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041718\
 Data File : BF104584.D
 Acq On : 18 Apr 2018 1:27
 Operator : JU/SJ
 Sample : J2410-05
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 T-3

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-BF040618.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	3.481	232	237	247	rVB	35613	56600	1.81%	0.214%
2	4.387	385	391	395	rBV	1909570	2556370	81.97%	9.651%
3	5.028	491	500	503	rBV	1807725	2667889	85.55%	10.072%
4	5.416	562	566	577	rVB	897885	775008	24.85%	2.926%
5	6.045	668	673	679	rVB	25927	39205	1.26%	0.148%
6	6.439	735	740	753	rBV	2058808	2066081	66.25%	7.800%
7	6.569	758	762	766	rBV	1355963	1101782	35.33%	4.159%
8	6.804	798	802	805	rBV	998944	832477	26.69%	3.143%
9	6.957	824	828	832	rBV	2462852	2341948	75.10%	8.841%
10	7.122	853	856	861	rBV	76945	67330	2.16%	0.254%
11	7.369	893	898	901	rBV	1949799	1790553	57.42%	6.760%
12	8.086	1016	1020	1023	rBV	1334869	1082514	34.71%	4.087%
13	9.163	1198	1203	1206	rBV	3502577	3118603	100.00%	11.773%
14	9.557	1265	1270	1273	rBV	307497	262007	8.40%	0.989%
15	9.769	1303	1306	1309	rVB	83601	62449	2.00%	0.236%
16	9.839	1315	1318	1322	rBV	1144171	1081831	34.69%	4.084%
17	10.269	1388	1391	1393	rVB	109963	80694	2.59%	0.305%
18	10.486	1422	1428	1431	rBV	75120	97516	3.13%	0.368%
19	10.627	1450	1452	1458	rBV	177234	169381	5.43%	0.639%
20	10.751	1469	1473	1477	rBV	151032	220653	7.08%	0.833%
21	11.104	1530	1533	1535	rBV	46549	36513	1.17%	0.138%
22	11.222	1549	1553	1559	rVB	191815	182947	5.87%	0.691%
23	11.327	1568	1571	1575	rBV	990309	923469	29.61%	3.486%
24	11.569	1610	1612	1615	rVB	87307	76499	2.45%	0.289%
25	12.310	1735	1738	1742	rBV	81533	94095	3.02%	0.355%
26	12.521	1771	1774	1777	rBV2	83665	108104	3.47%	0.408%
27	12.921	1836	1842	1845	rBV	2402348	2269411	72.77%	8.568%
28	13.774	1985	1987	1990	rBV	97553	94779	3.04%	0.358%
29	13.810	1990	1993	2000	rVB	424995	435702	13.97%	1.645%
30	13.974	2018	2021	2025	rVB	882652	774597	24.84%	2.924%
31	14.104	2040	2043	2046	rBV	60551	63965	2.05%	0.241%
32	14.145	2047	2050	2053	rVB	112622	93603	3.00%	0.353%
33	14.445	2099	2101	2105	rVB2	32760	36306	1.16%	0.137%
34	14.821	2162	2165	2168	rVB	40664	40437	1.30%	0.153%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.433	2264	2269	2278	rBV	473885	625093	20.04%	2.360%
36	15.886	2342	2346	2349	rBV2	28121	38873	1.25%	0.147%
37	15.933	2350	2354	2363	rVB2	53266	86722	2.78%	0.327%
38	16.962	2526	2529	2537	rVB7	17747	36416	1.17%	0.137%

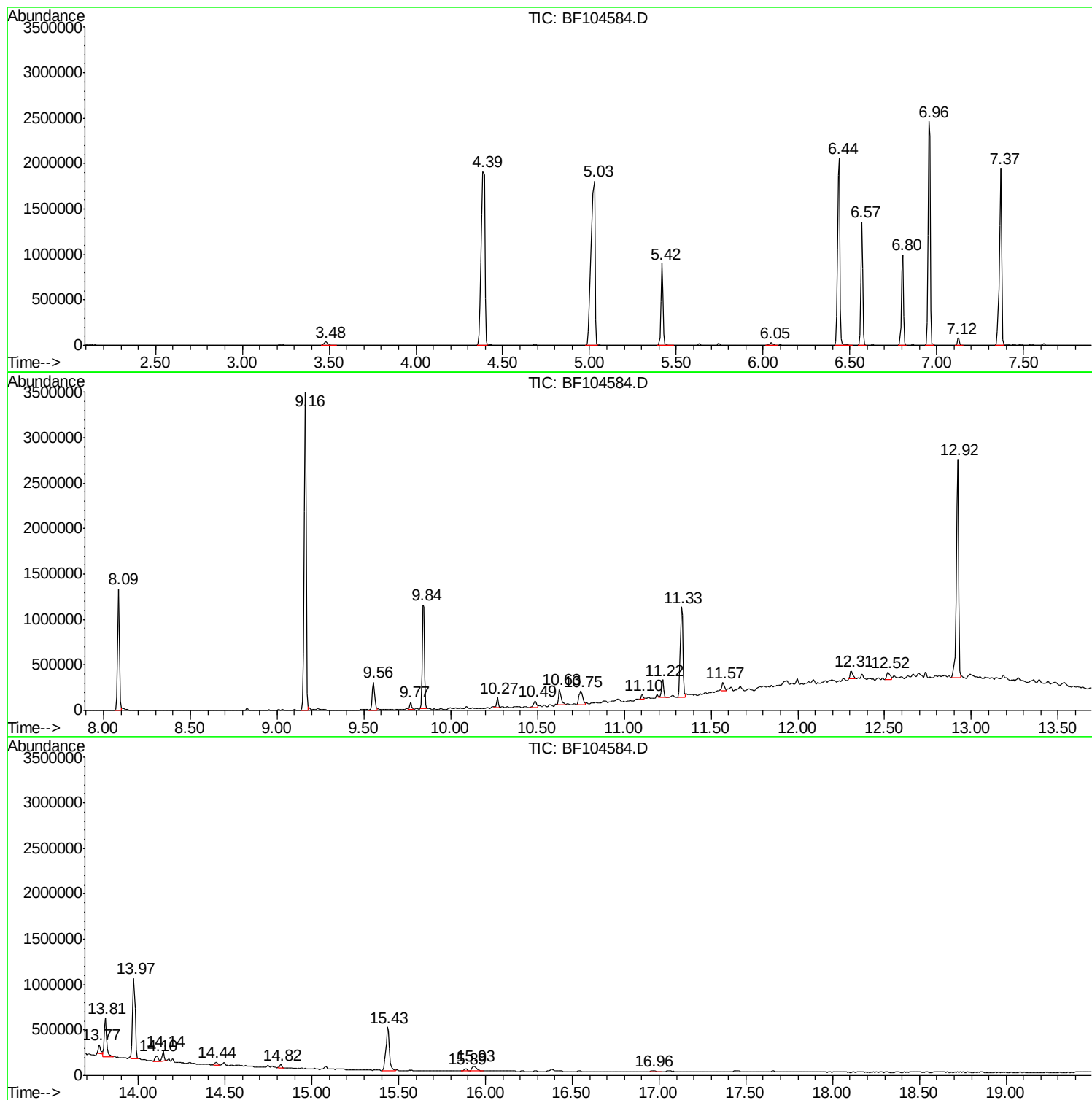
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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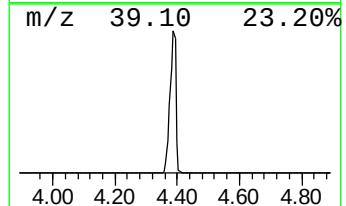
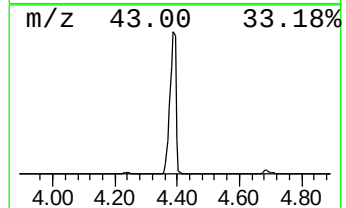
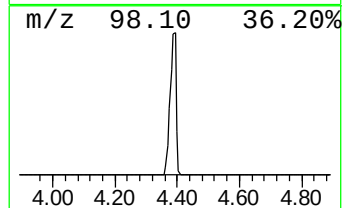
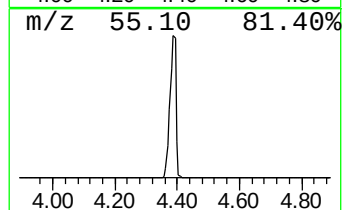
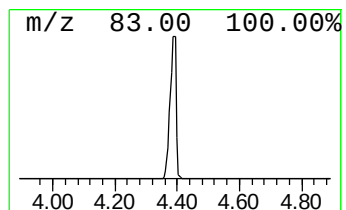
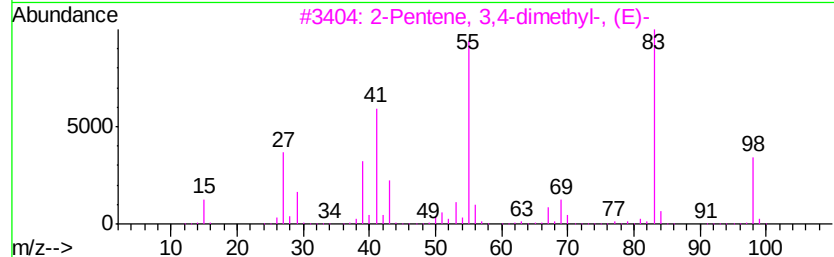
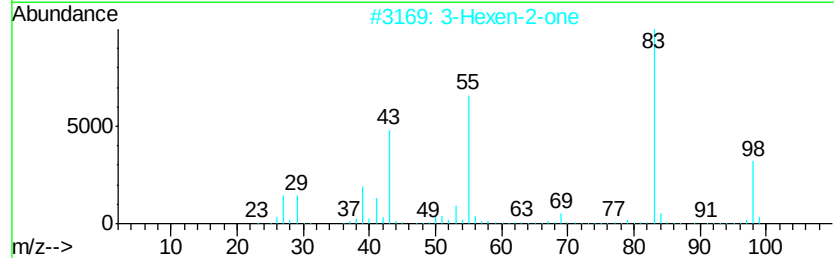
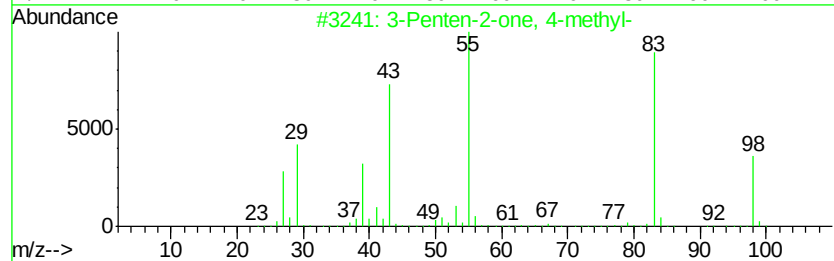
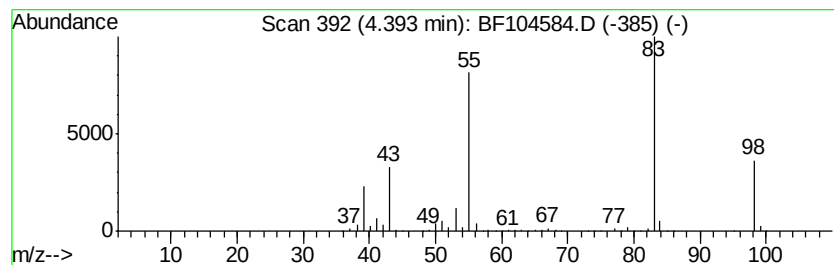
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	61.42 ng	2556370	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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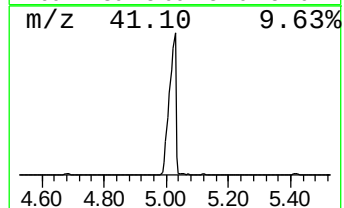
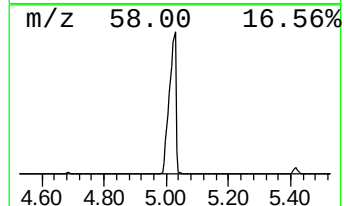
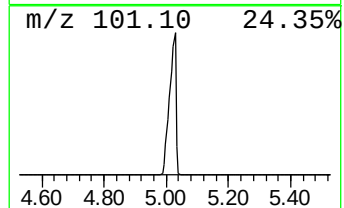
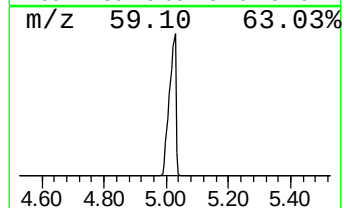
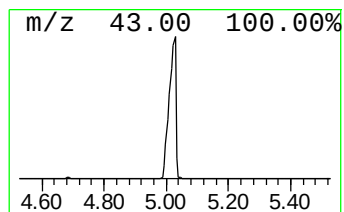
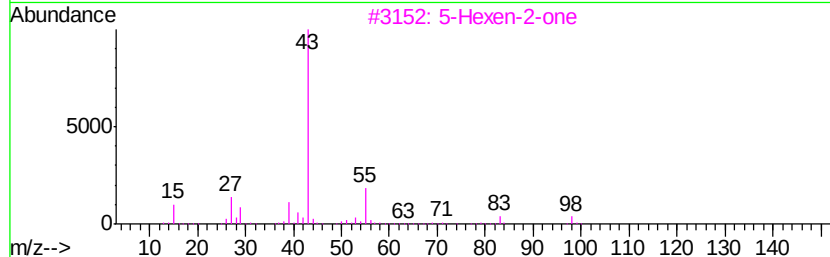
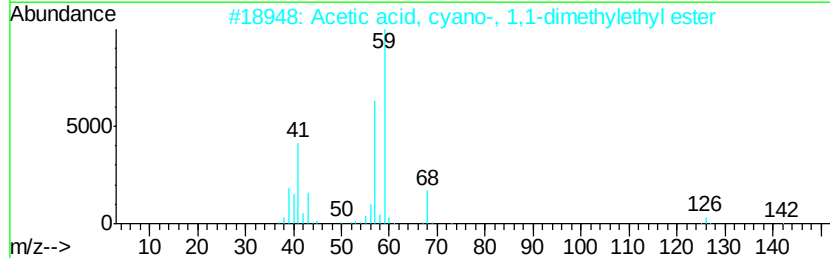
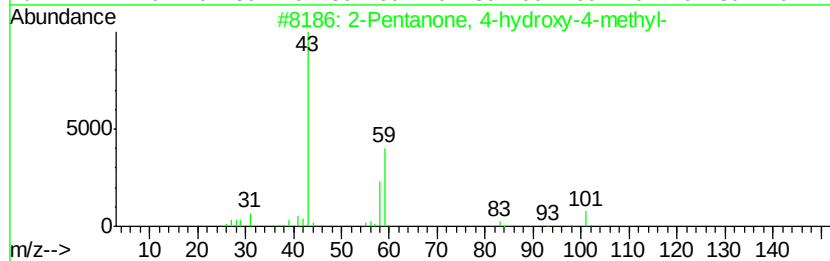
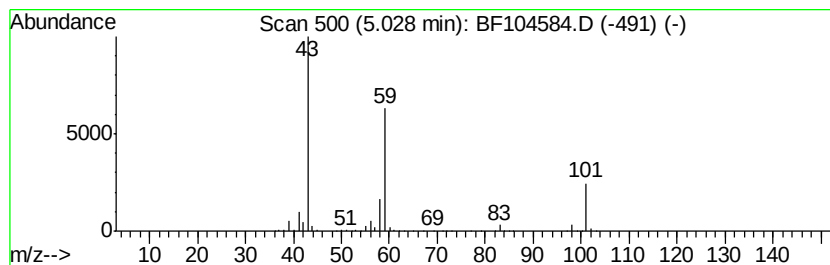
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	64.10 ng	2667890	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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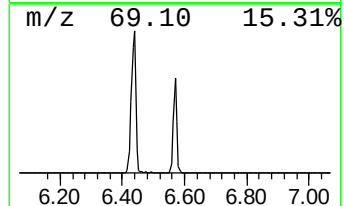
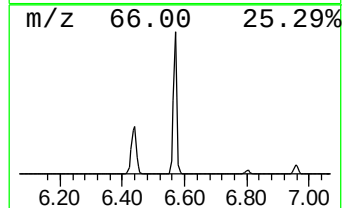
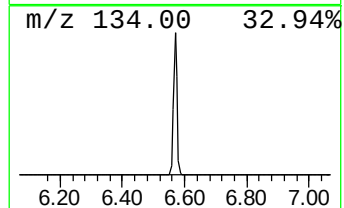
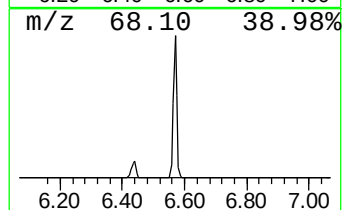
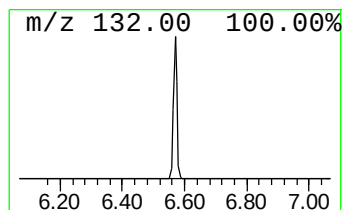
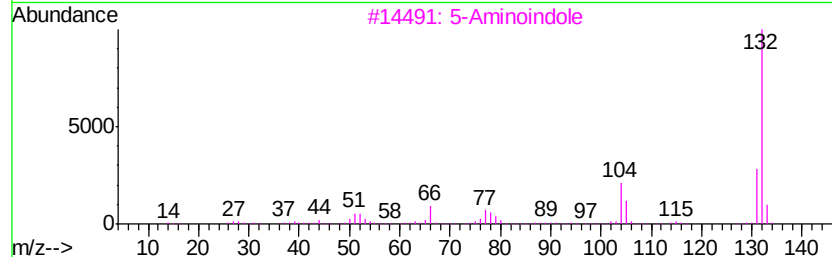
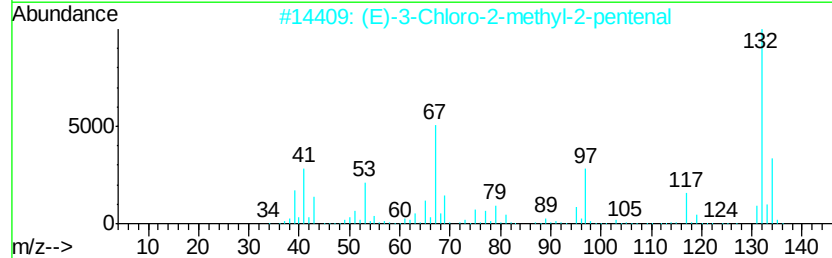
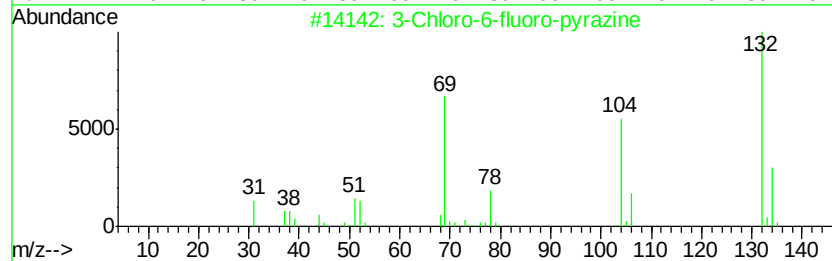
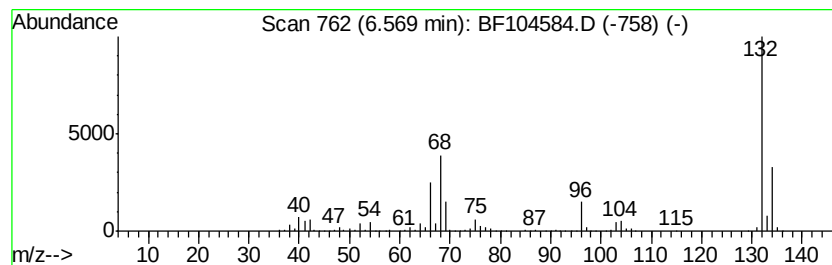
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.57 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	26.47 ng	1101780	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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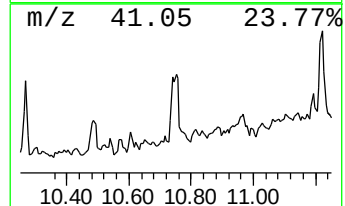
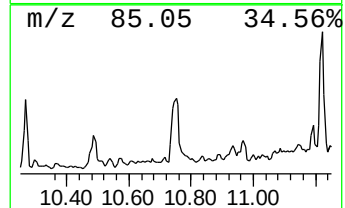
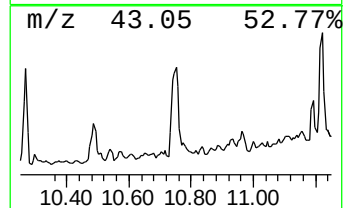
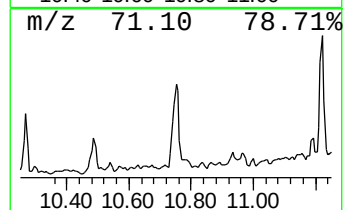
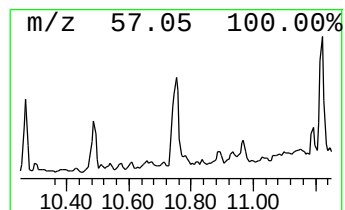
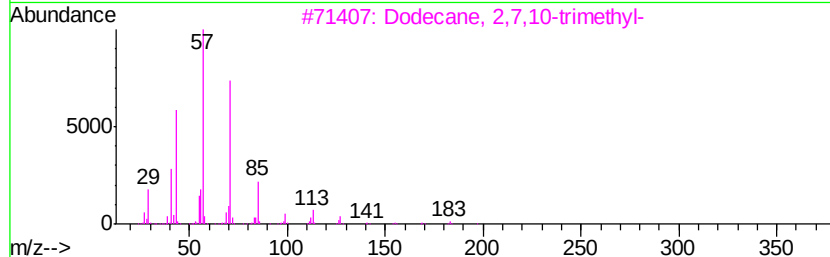
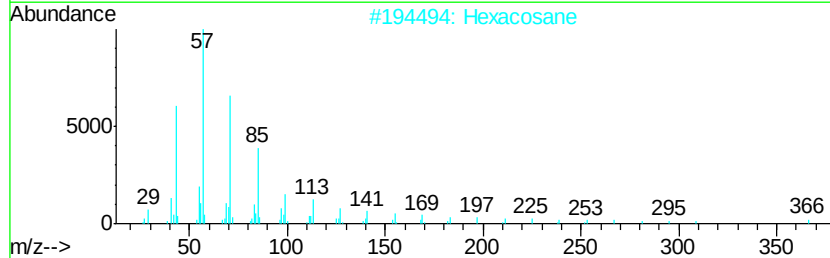
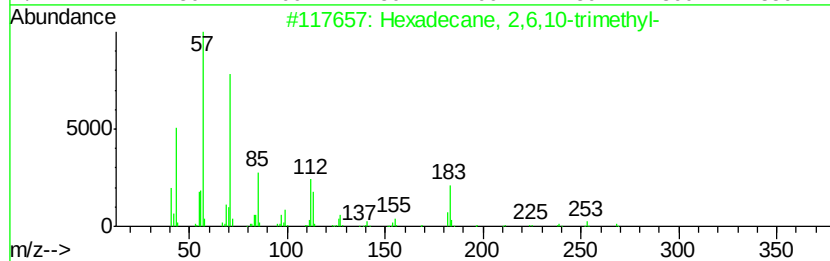
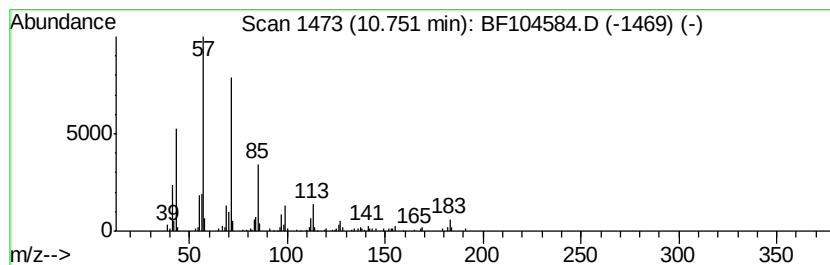
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecane, 2,6,10-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	4.78 ng	220653	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 2,6,10-trimethyl-	268	C19H40	055000-52-7	90
2		Hexacosane	366	C26H54	000630-01-3	86
3		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	86
4		Heptacosane	380	C27H56	000593-49-7	86
5		Octane, 2-methyl-	128	C9H20	003221-61-2	81



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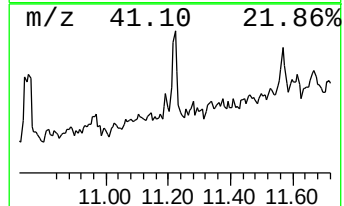
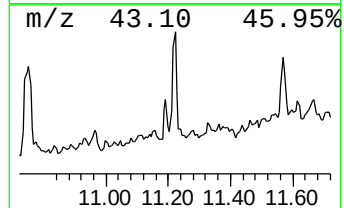
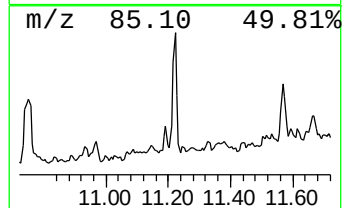
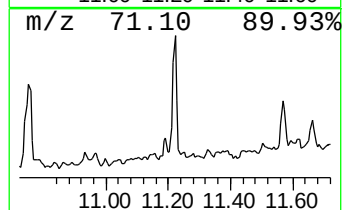
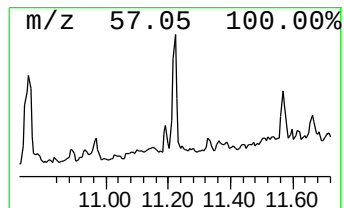
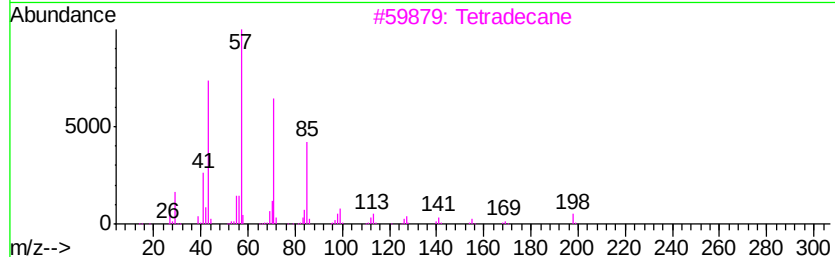
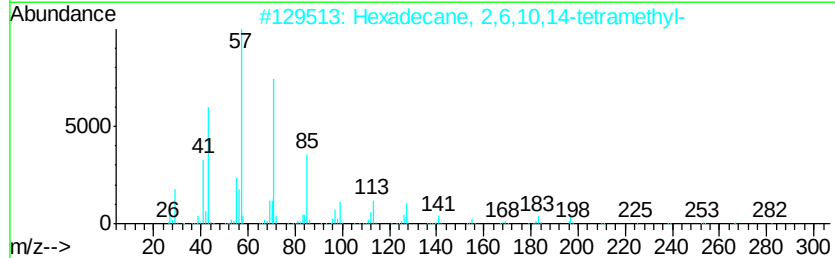
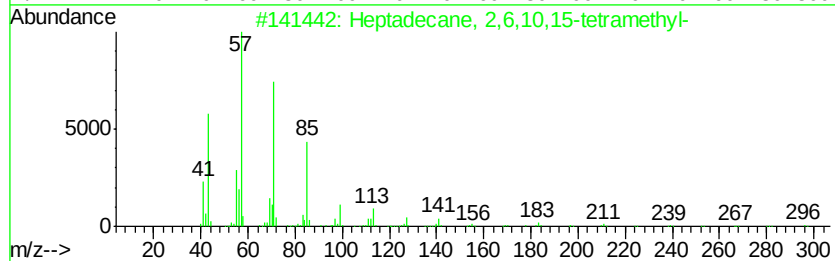
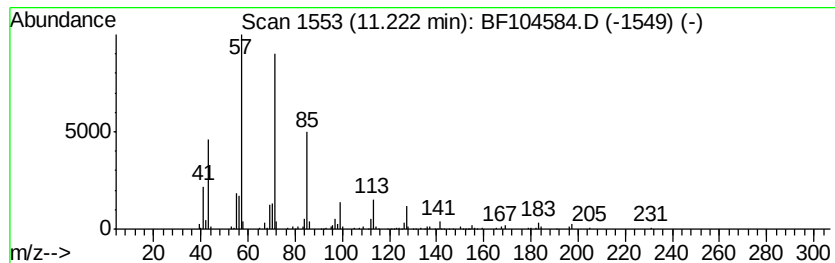
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecane, 2,6,10,15-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	3.96 ng	182947	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
2		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	83
3		Tetradecane	198	C14H30	000629-59-4	78
4		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
5		Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	58



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Operator : JU/SJ
Sample : J2410-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

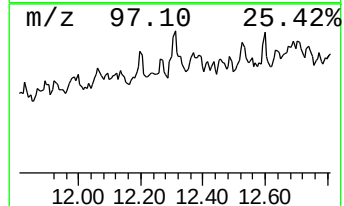
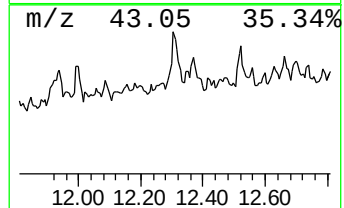
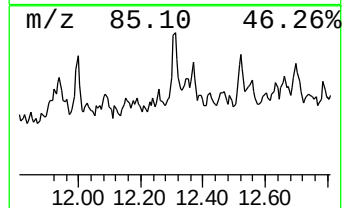
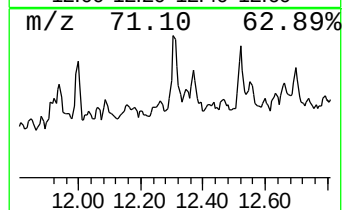
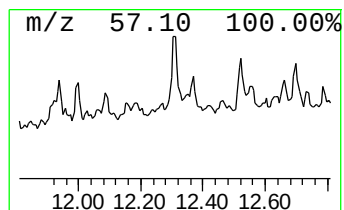
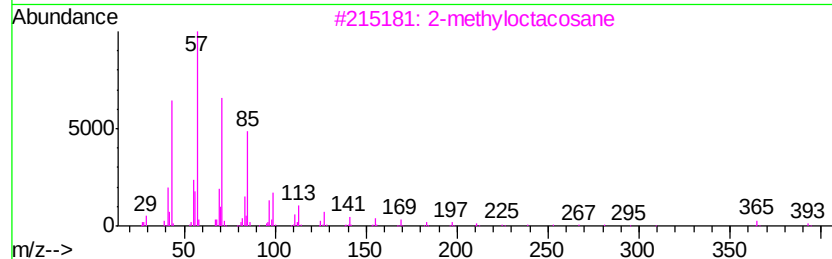
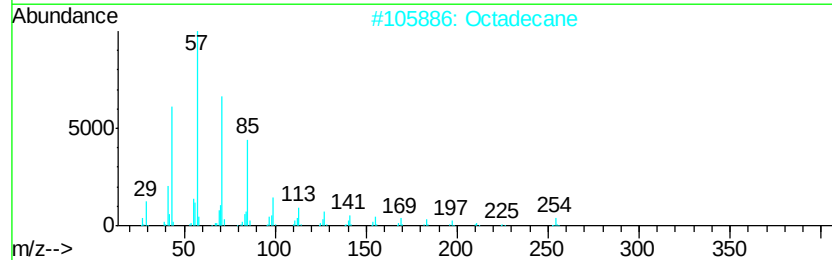
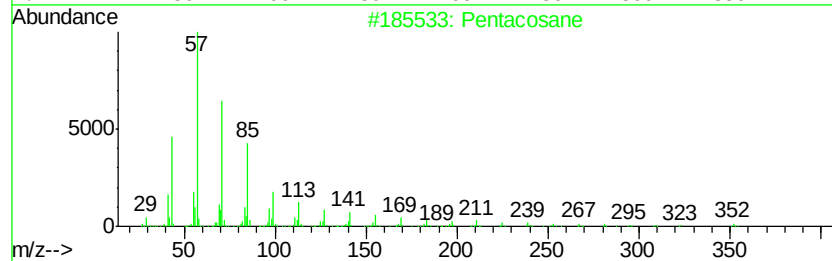
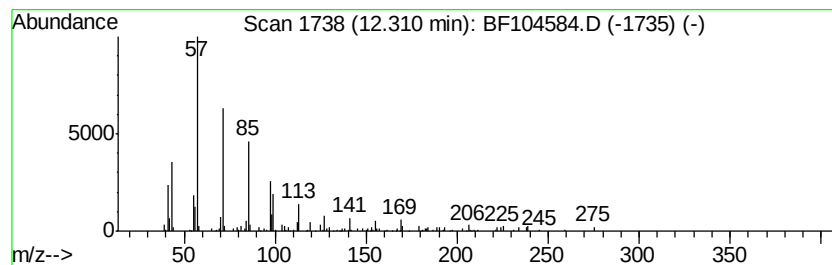
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	2.04 ng	94095	Phenanthrene-d10	11.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	80
2	Octadecane	254 C18H38	000593-45-3	72
3	2-methyloctacosane	408 C29H60	1000376-72-8	72
4	triacontane	422 C30H62	000638-68-6	72
5	Tetracosane	338 C24H50	000646-31-1	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041718\
Data File : BF104584.D
Acq On : 18 Apr 2018 1:27
Operator : JU/SJ
Sample : J2410-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

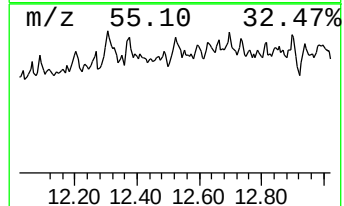
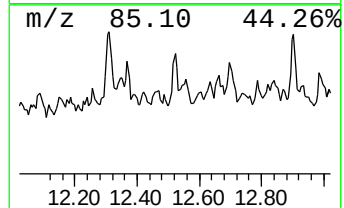
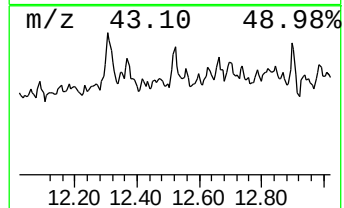
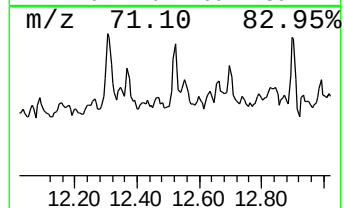
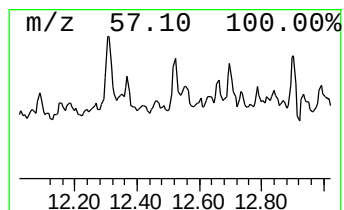
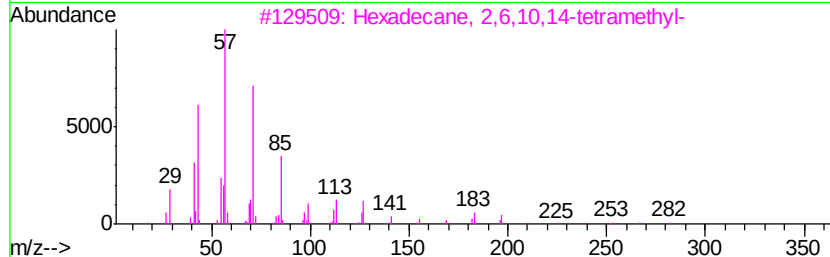
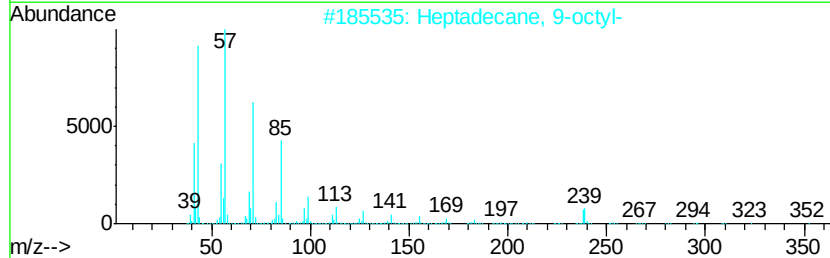
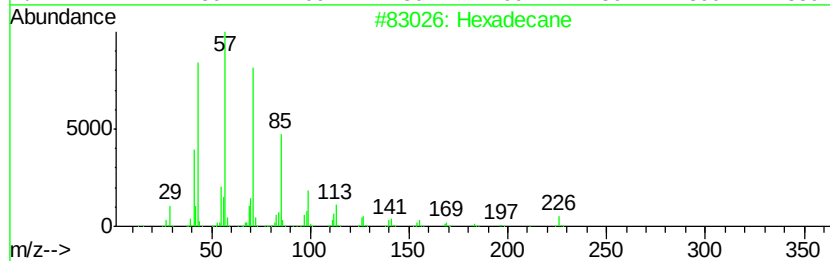
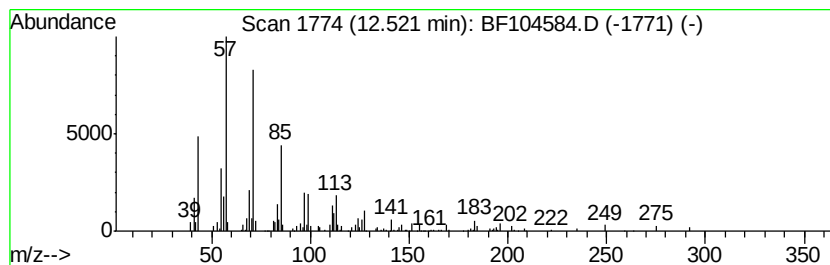
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ClientSampleId :
T-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	2.34 ng	108104	Phenanthrene-d10	11.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	80
2	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	80
3	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	80
4	Eicosane, 7-hexyl-	366 C26H54	055333-99-8	80
5	Hentriacontane	437 C31H64	000630-04-6	78



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041718\
Data File : BF104584.D
Acq On : 18 Apr 2018 1:27
Operator : JU/SJ
Sample : J2410-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
T-3

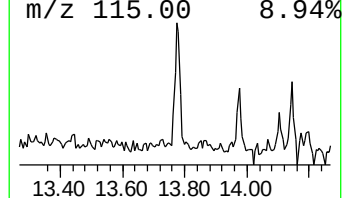
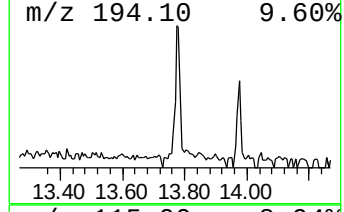
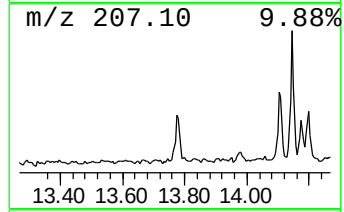
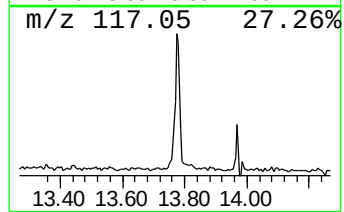
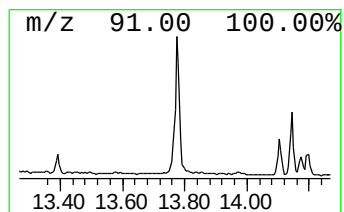
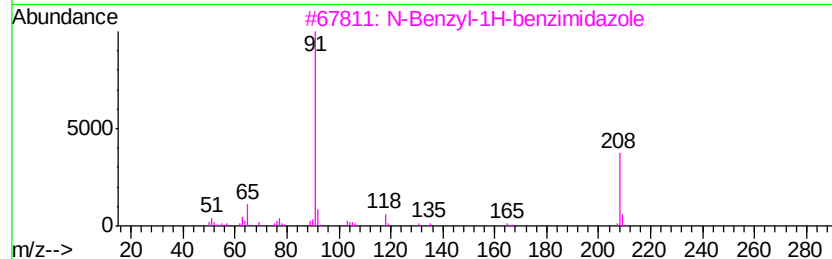
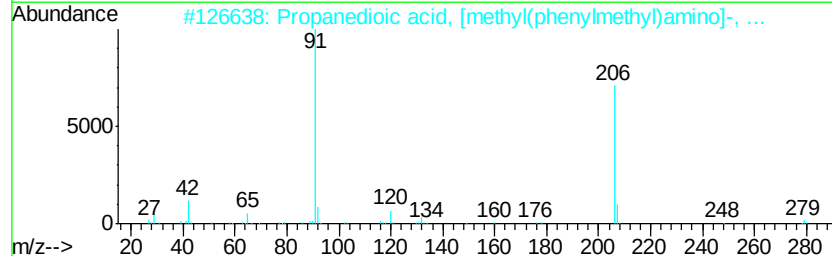
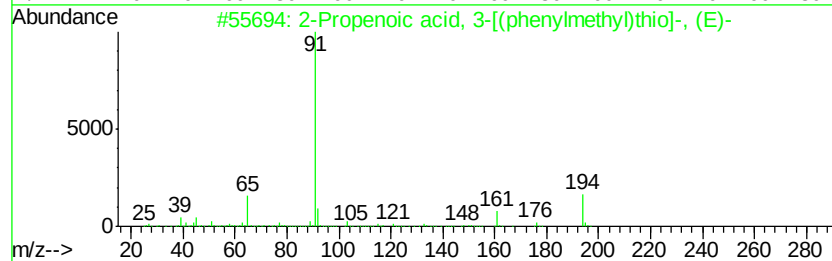
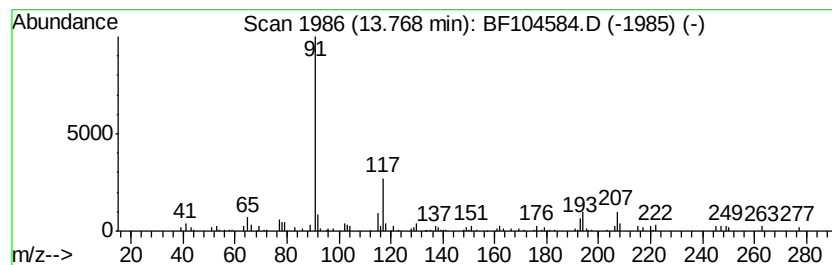
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.77 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.45 ng	94779	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	16
2		Propanedioic acid, [methyl(pheny...	279	C15H21N04	001032-02-6	12
3		N-Benzyl-1H-benzimidazole	208	C14H12N2	004981-92-4	12
4		Methoxyacetic acid, benzyl ester	180	C10H12O3	032786-24-6	11
5		L-(-)-Fucose, tetrakis(trifluoro...	653	C21H15F12N09	1000380-45-2	10



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041718\
Data File : BF104584.D
Acq On : 18 Apr 2018 1:27
Operator : JU/SJ
Sample : J2410-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

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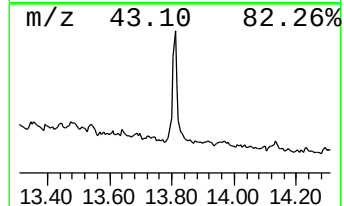
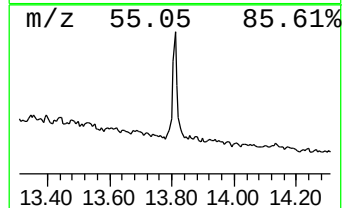
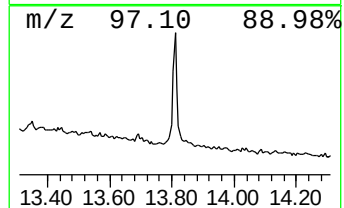
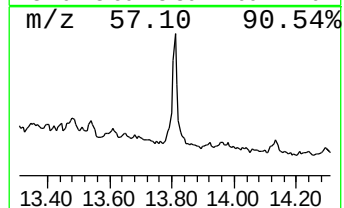
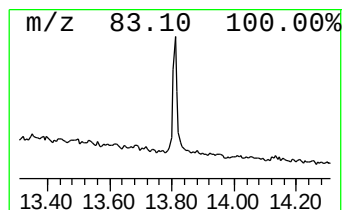
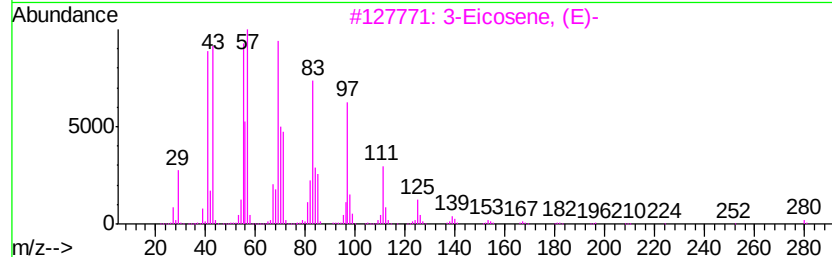
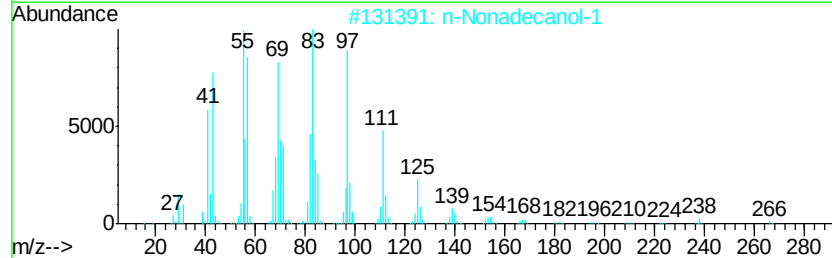
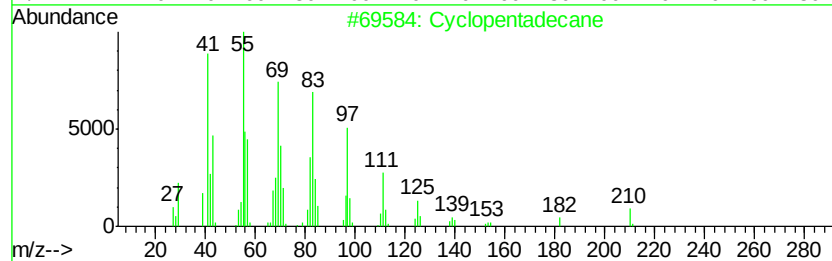
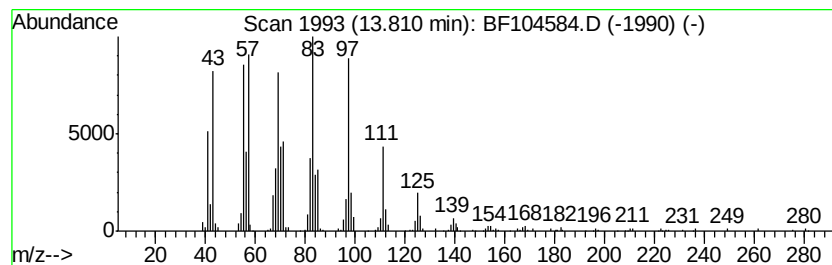
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	11.25 ng	435702	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	93
2		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5		Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF041718\
Data File : BF104584.D
Acq On : 18 Apr 2018 1:27
Operator : JU/SJ
Sample : J2410-05
Misc :
ALS Vial : 25 Sample Multiplier: 1

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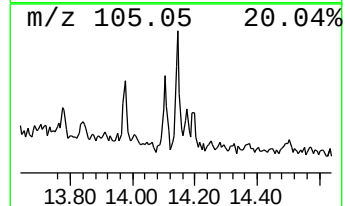
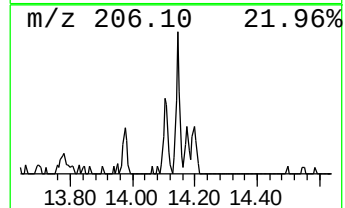
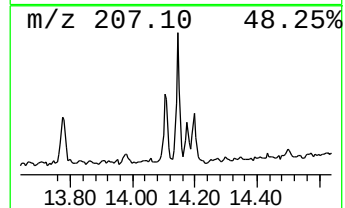
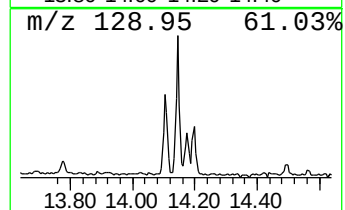
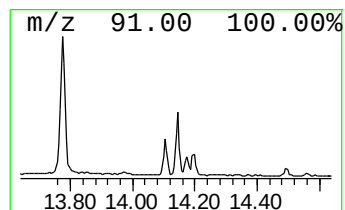
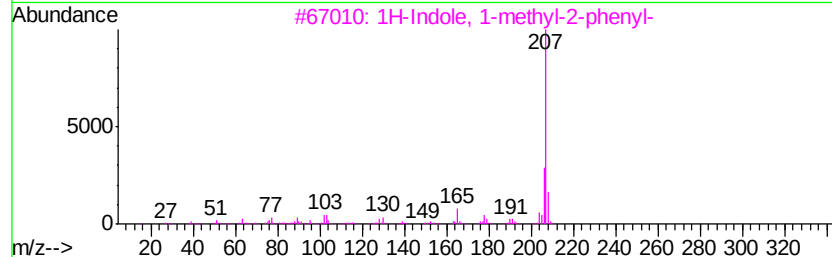
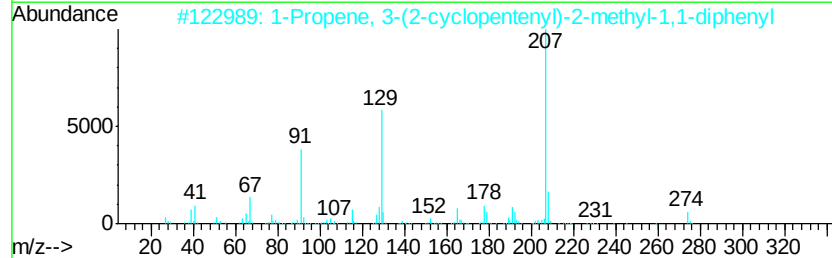
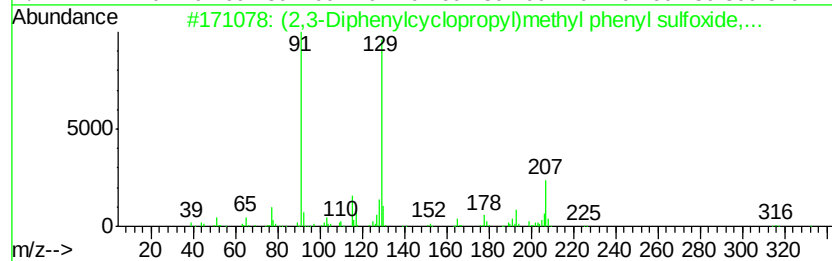
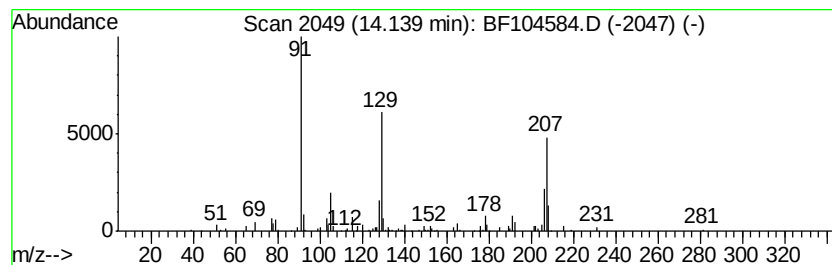
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 (2,3-Diphenylcyclopropyl)me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.42 ng	93603	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	64
2		1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	50
3		1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	41
4		5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	35
5		1-benzylindole	207	C15H13N	1000334-31-3	32



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041718\
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Sample : J2410-05
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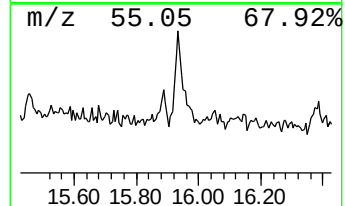
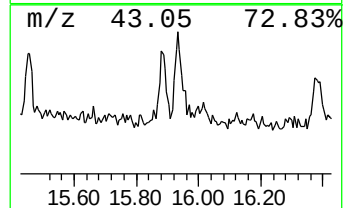
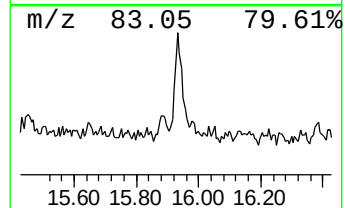
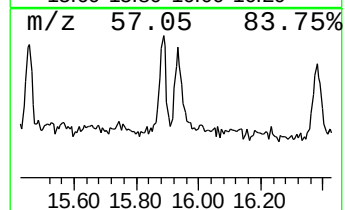
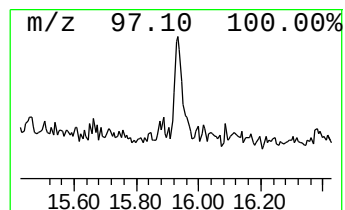
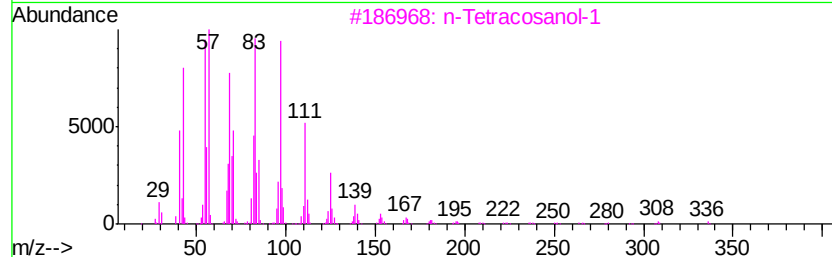
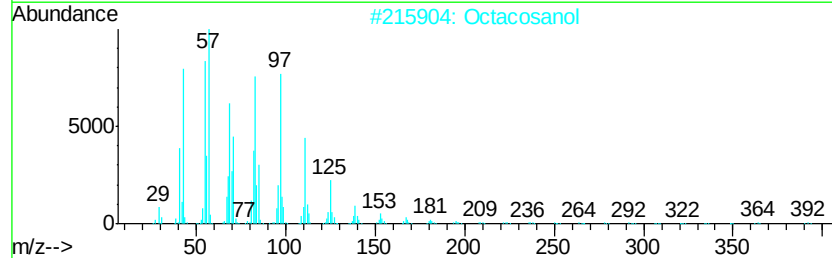
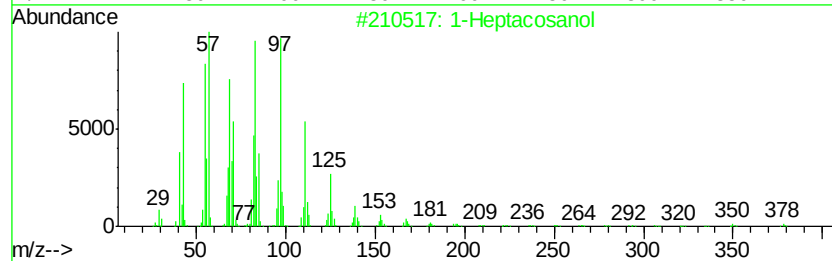
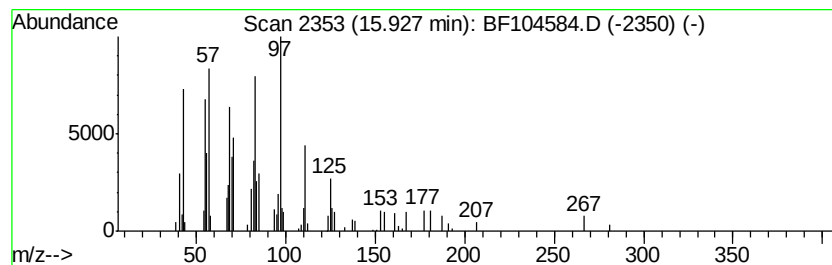
Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.93	2.77 ng	86722	Perylene-d12		15.43
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	Octacosanol	410	C28H58O	000557-61-9	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
4	Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
5	Octacosyl acetate	452	C30H60O2	018206-97-8	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041718\
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 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.03	64.1	ng	2667890	1	6.80	832477	20.0
unknown6.57	6.57	26.5	ng	1101780	1	6.80	832477	20.0
Hexadecane, 2,6,1...	10.75	4.8	ng	220653	4	11.33	923469	20.0
Heptadecane, 2,6,...	11.22	4.0	ng	182947	4	11.33	923469	20.0
Pentacosane	12.31	2.0	ng	94095	4	11.33	923469	20.0
Hexadecane	12.52	2.3	ng	108104	4	11.33	923469	20.0
unknown13.77	13.77	2.5	ng	94779	5	13.97	774597	20.0
Cyclopentadecane	13.81	11.3	ng	435702	5	13.97	774597	20.0
(2,3-Diphenylcycl...	14.14	2.4	ng	93603	5	13.97	774597	20.0
1-Heptacosanol	15.93	2.8	ng	86722	6	15.43	625093	20.0