

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101618\
 Data File : BF109906.D
 Acq On : 16 Oct 2018 15:40
 Operator : JU/SJ
 Sample : J5526-14
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SUP-4B-C-101518-3

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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	2.328	36	41	47	rVB	729762	987232	19.86%	2.034%
2	3.587	252	255	269	rBV	85284	167758	3.37%	0.346%
3	5.222	528	533	538	rVB	181101	205972	4.14%	0.424%
4	5.604	593	598	601	rBV	4991311	4789318	96.33%	9.870%
5	6.598	762	767	771	rBV	4958647	4971787	100.00%	10.246%
6	6.751	788	793	796	rBV	5180512	4893494	98.43%	10.084%
7	6.981	828	832	835	rVB	1918430	1499179	30.15%	3.089%
8	7.140	855	859	862	rVB	4362635	3860670	77.65%	7.956%
9	7.540	922	927	930	rBV	3345500	3065717	61.66%	6.318%
10	8.263	1046	1050	1053	rBV	2265800	1816681	36.54%	3.744%
11	9.339	1228	1233	1236	rVB	4873393	4509530	90.70%	9.293%
12	9.728	1295	1299	1302	rVB	596570	477028	9.59%	0.983%
13	10.022	1345	1349	1353	rBV	1977703	1646266	33.11%	3.393%
14	10.810	1479	1483	1486	rBV	2495164	2074424	41.72%	4.275%
15	11.510	1599	1602	1605	rBV	1485527	1346162	27.08%	2.774%
16	11.533	1605	1606	1611	rVB	120545	91801	1.85%	0.189%
17	11.722	1634	1638	1642	rBV2	59761	60265	1.21%	0.124%
18	12.016	1685	1688	1691	rBV2	89655	97187	1.95%	0.200%
19	12.539	1774	1777	1780	rBV	199524	168577	3.39%	0.347%
20	12.727	1805	1809	1813	rBV	415803	359543	7.23%	0.741%
21	12.804	1818	1822	1828	rBV5	46823	74011	1.49%	0.153%
22	12.957	1842	1848	1854	rVB	381165	392979	7.90%	0.810%
23	13.098	1868	1872	1875	rVB	3976311	3375219	67.89%	6.955%
24	13.657	1962	1967	1969	rBV2	64863	61841	1.24%	0.127%
25	13.974	2016	2021	2032	rVB6	389830	533880	10.74%	1.100%
26	14.157	2047	2052	2055	rBV	1914624	1920768	38.63%	3.958%
27	14.180	2055	2056	2062	rVB	217641	165291	3.32%	0.341%
28	14.298	2073	2076	2081	rBV	137998	137766	2.77%	0.284%
29	14.610	2126	2129	2136	rVB	268361	296075	5.96%	0.610%
30	14.704	2141	2145	2148	rBV5	43750	57069	1.15%	0.118%
31	14.774	2155	2157	2165	rVB8	34987	56360	1.13%	0.116%
32	14.927	2180	2183	2190	rVB	244700	280309	5.64%	0.578%
33	15.010	2194	2197	2201	rBV	91627	91665	1.84%	0.189%
34	15.227	2230	2234	2237	rBV	185401	269304	5.42%	0.555%

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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	15.286	2241	2244	2251	rVB	313828	379565	7.63%	0.782%
36	15.551	2285	2289	2294	rVV	103180	130993	2.63%	0.270%
37	15.615	2296	2300	2306	rBV	159480	201016	4.04%	0.414%
38	15.686	2307	2312	2322	rBV2	1524467	2152682	43.30%	4.436%
39	16.157	2388	2392	2397	rVV	258877	375506	7.55%	0.774%
40	16.210	2398	2401	2409	rVB3	75513	116819	2.35%	0.241%
41	16.704	2480	2485	2492	rVB2	139797	256425	5.16%	0.528%
42	17.245	2573	2577	2583	rVB3	55776	111769	2.25%	0.230%

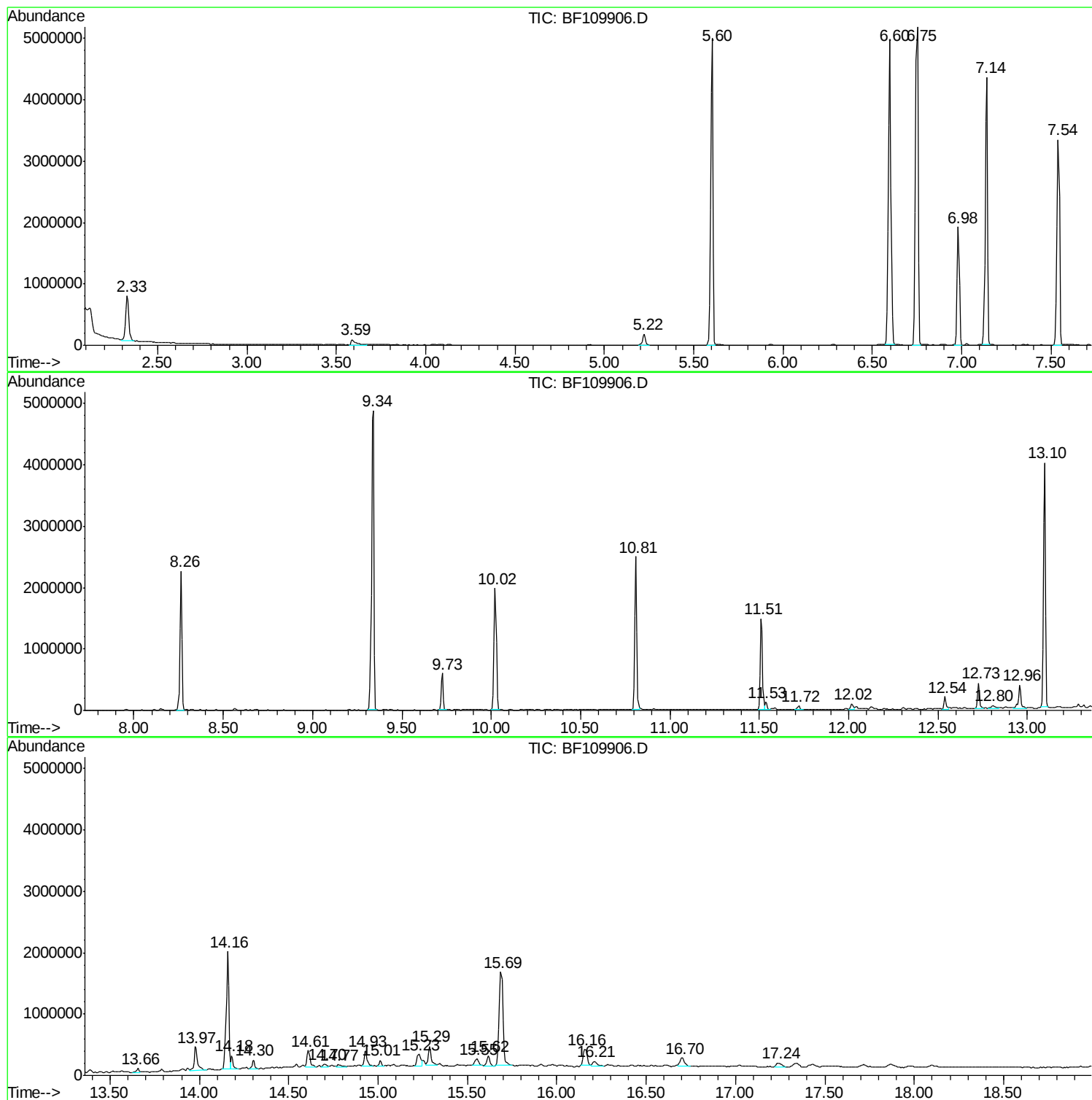
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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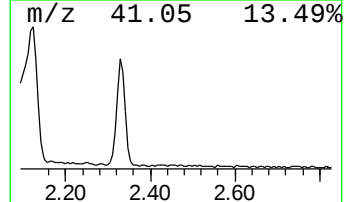
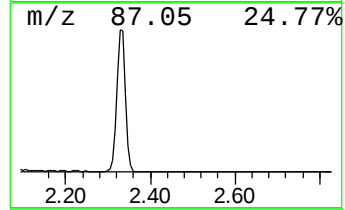
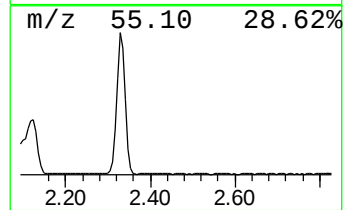
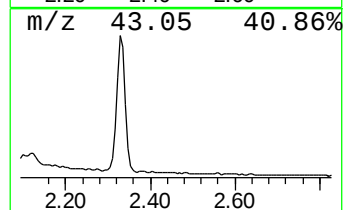
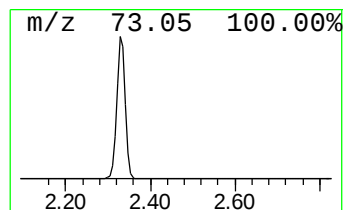
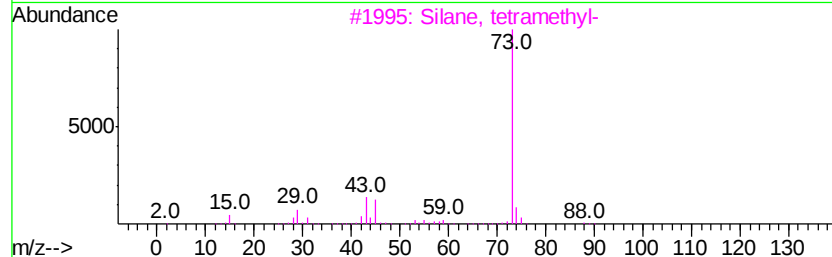
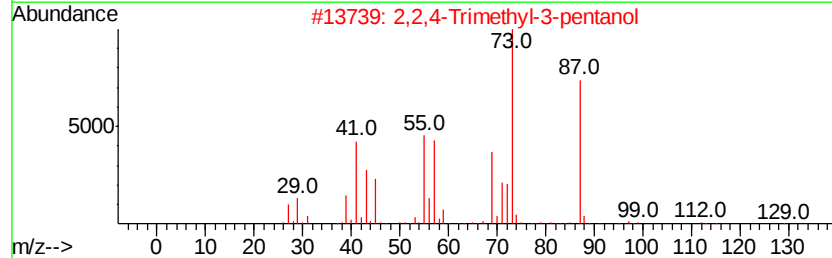
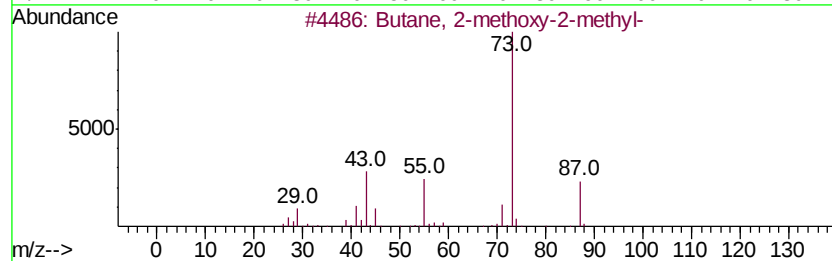
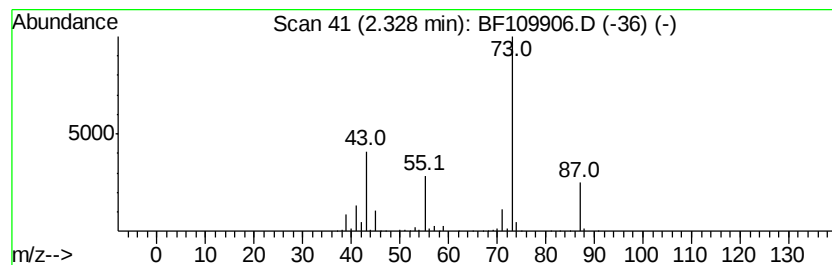
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	13.17 ng	987232	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25



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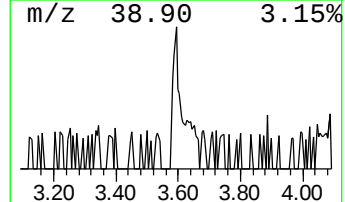
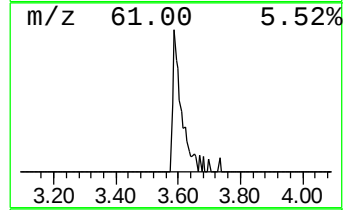
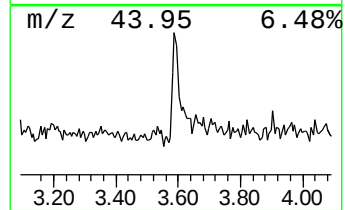
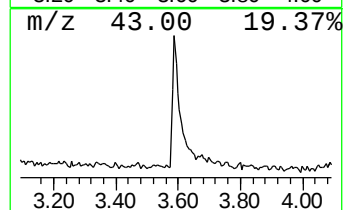
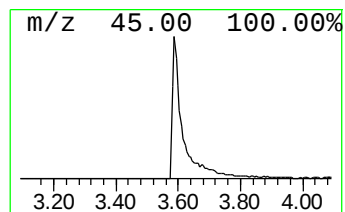
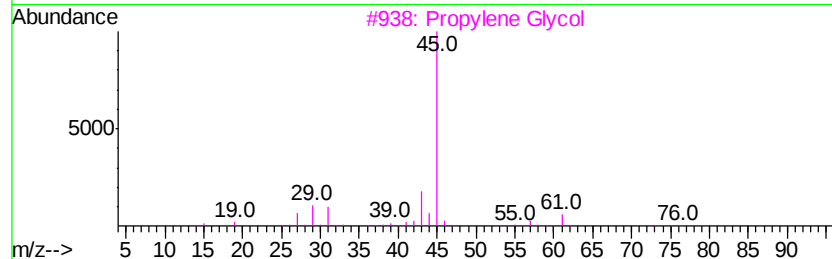
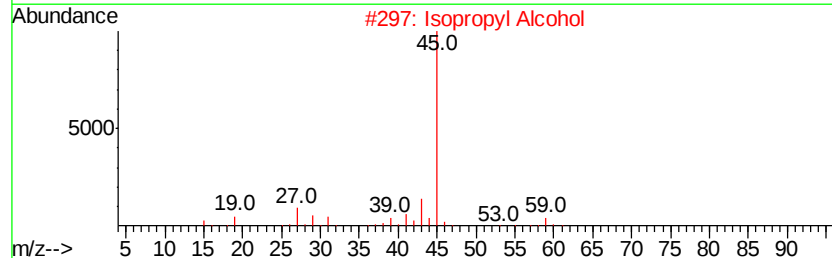
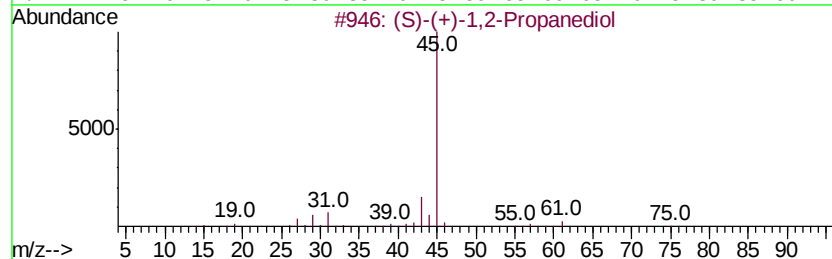
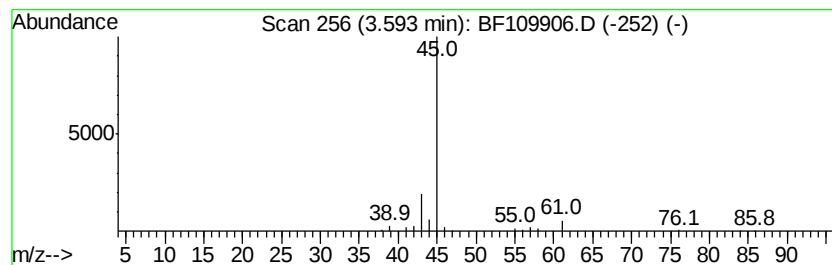
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (S)-(+)-1,2-Propanediol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.59	2.24 ng	167758	1,4-Dichlorobenzene-d4	6.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3		Propylene Glycol	76	C3H8O2	000057-55-6	43
4		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
5		Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9



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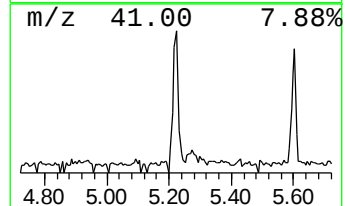
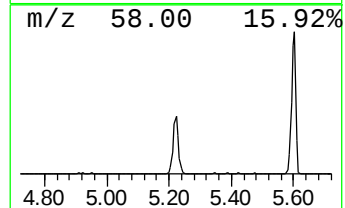
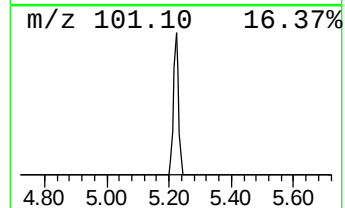
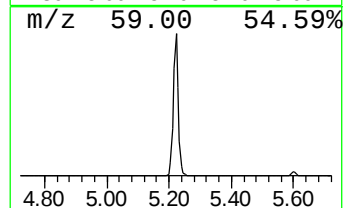
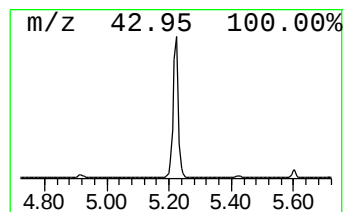
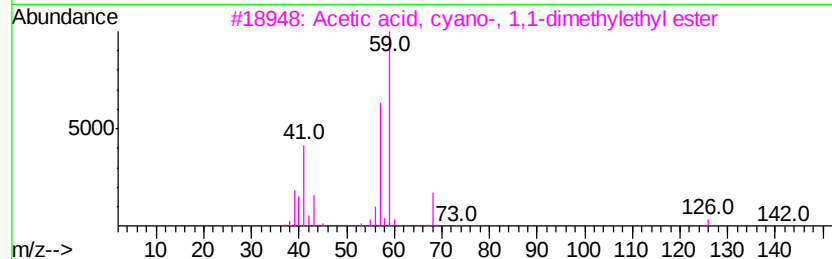
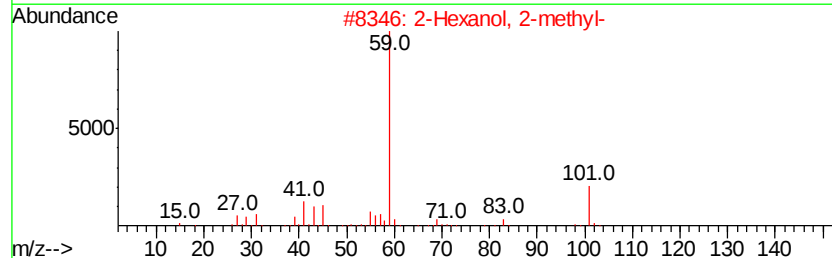
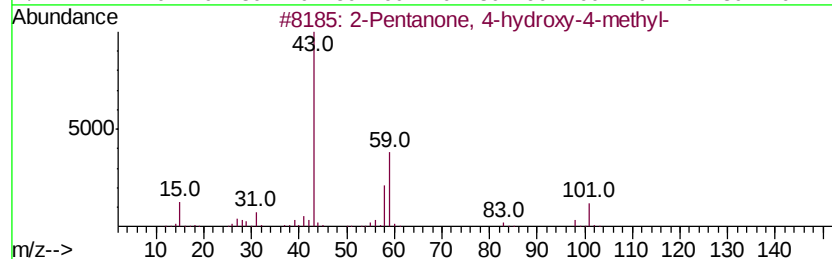
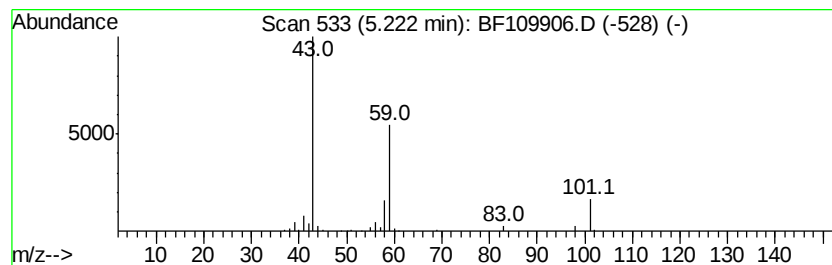
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.22	2.75 ng	205972	1,4-Dichlorobenzene-d4	6.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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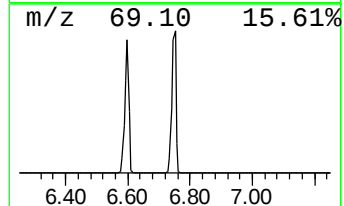
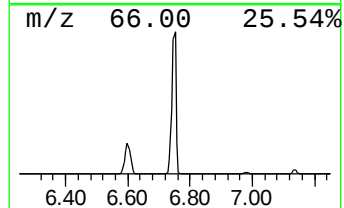
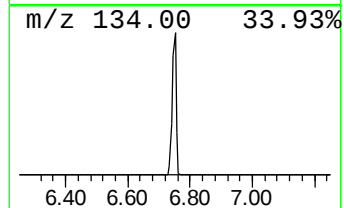
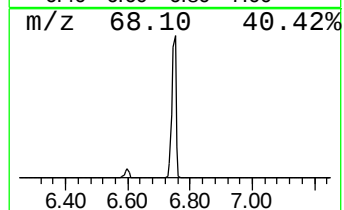
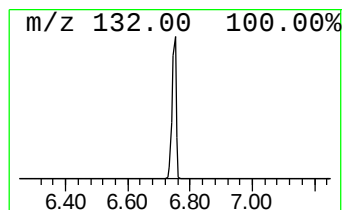
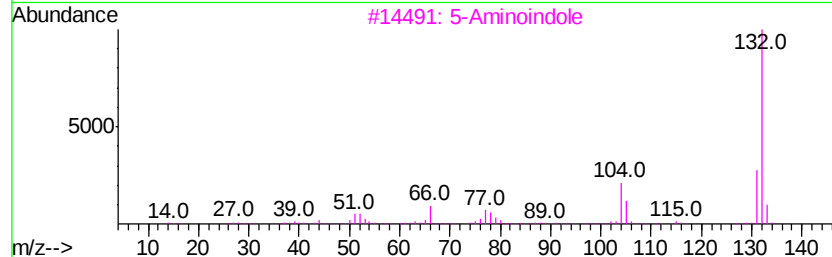
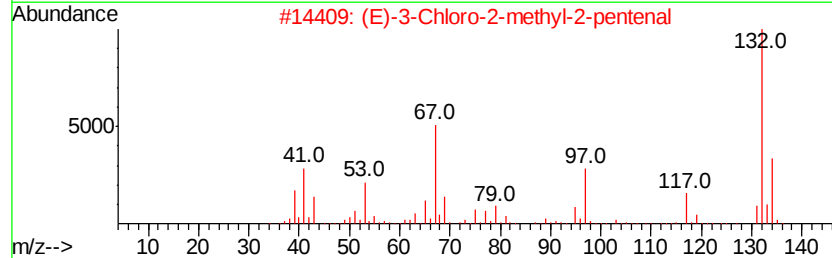
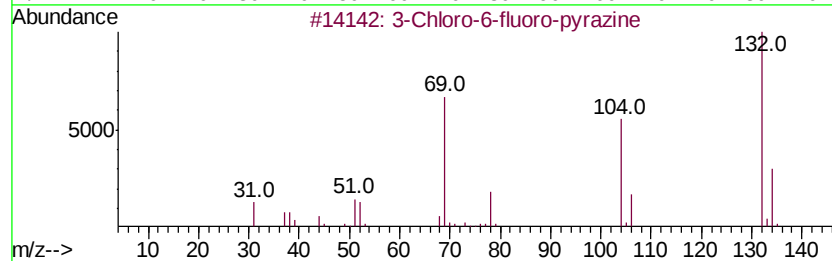
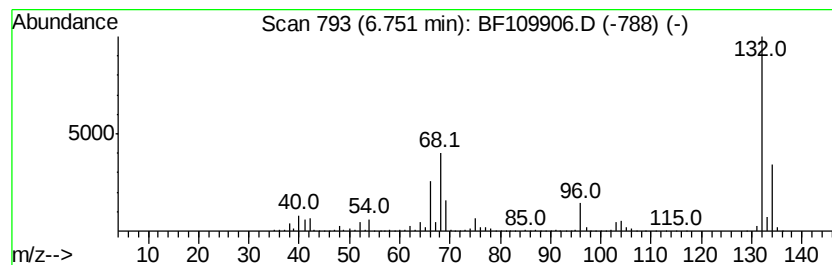
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	65.28 ng	4893490	1,4-Dichlorobenzene-d4	6.98

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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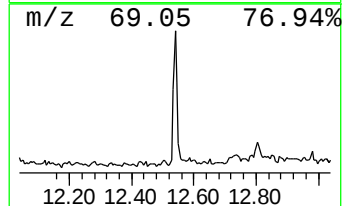
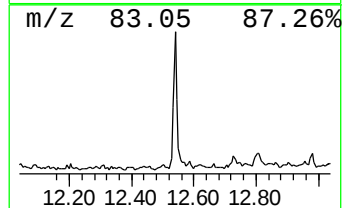
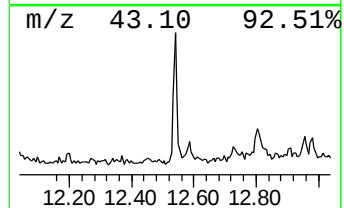
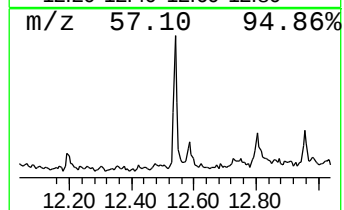
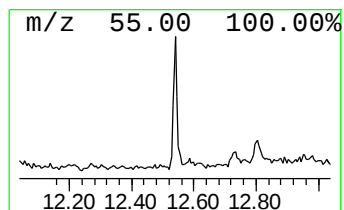
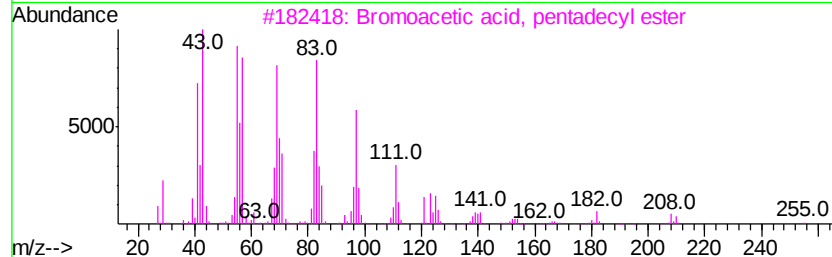
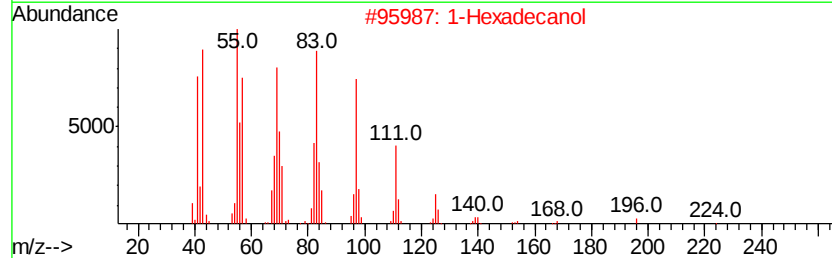
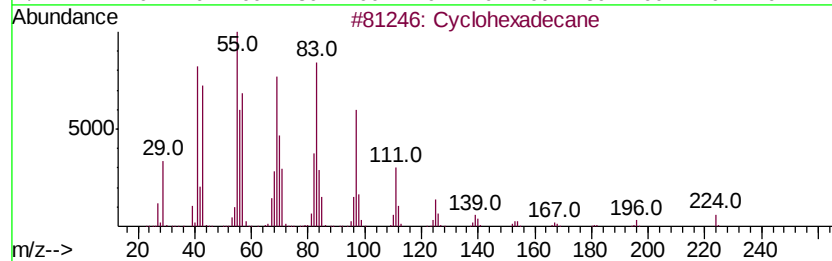
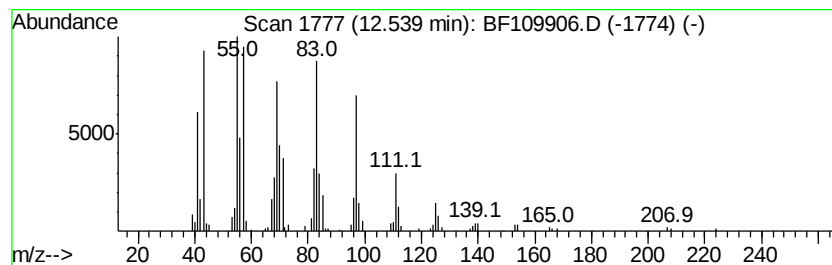
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	2.50 ng	168577	Phenanthrene-d10	11.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			1-Hexadecanol	242	C16H34O	036653-82-4	94
3			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
4			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5			9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
Operator : JU/SJ
Sample : J5526-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SUP-4B-C-101518-3

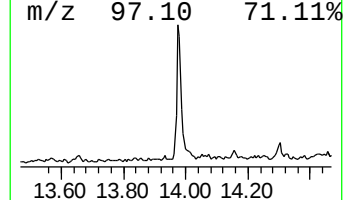
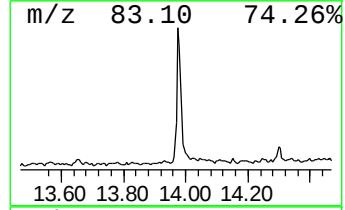
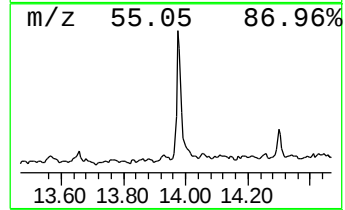
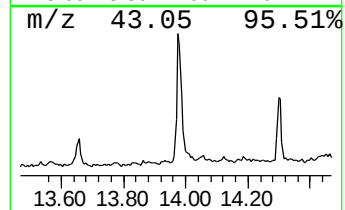
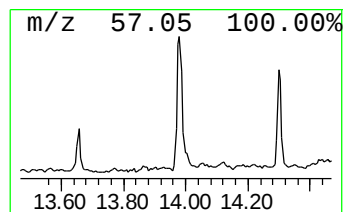
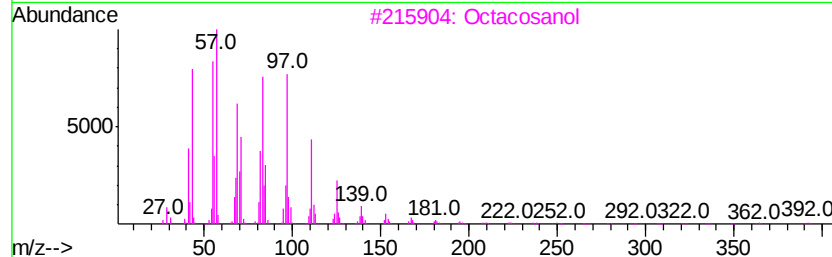
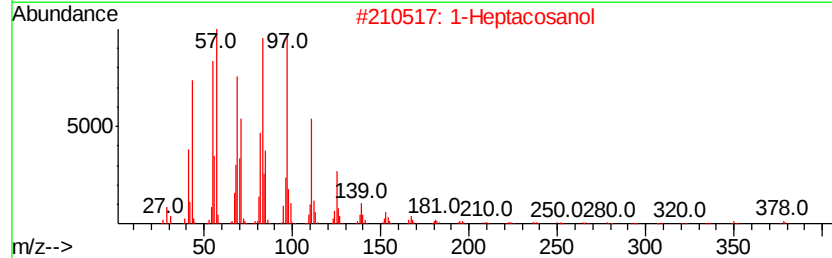
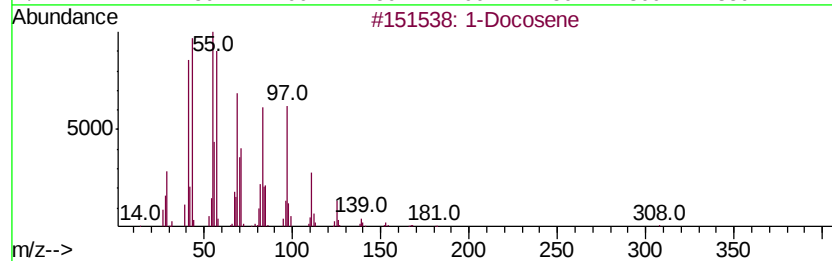
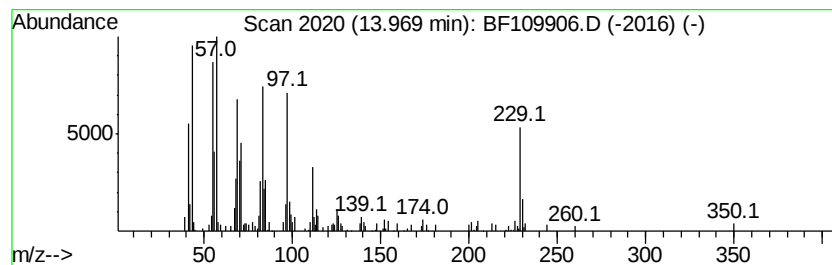
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.56 ng	533880	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	91
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Octacosanol	410	C28H58O	000557-61-9	91
4		Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
Operator : JU/SJ
Sample : J5526-14
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Instrument :
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ClientSampleId :
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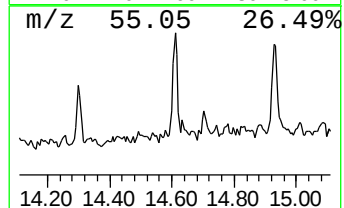
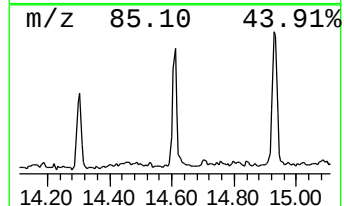
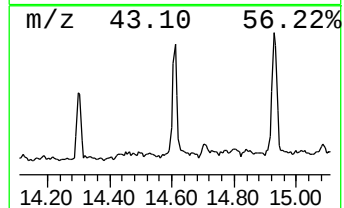
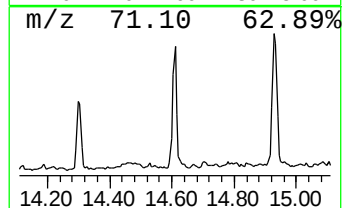
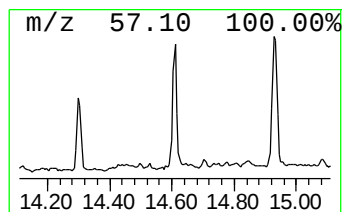
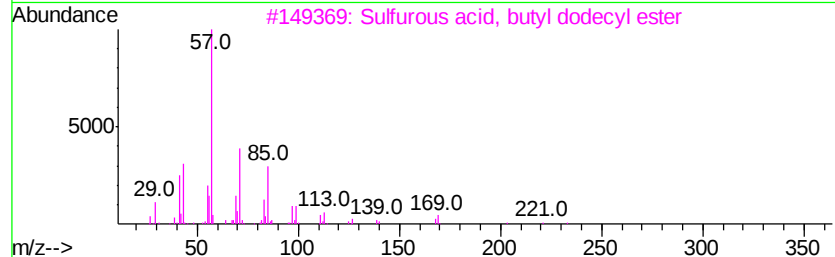
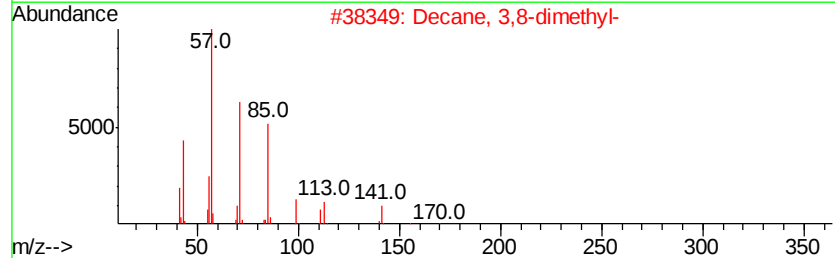
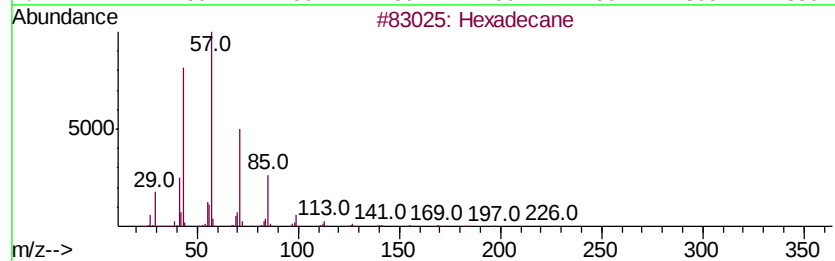
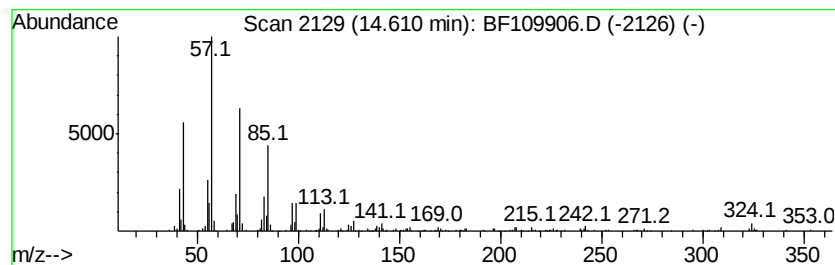
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.61	3.08 ng	296075	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	95
2		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	91
3		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	90
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
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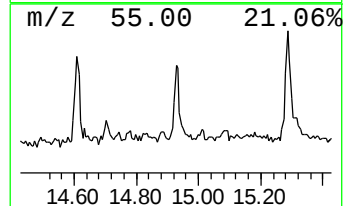
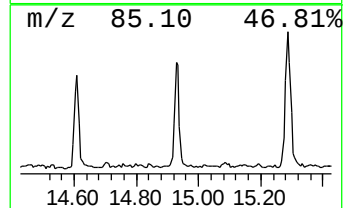
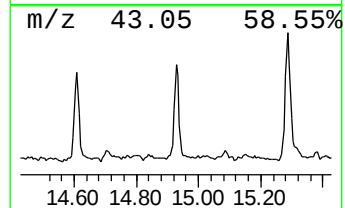
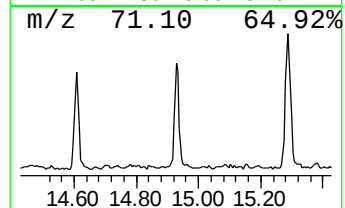
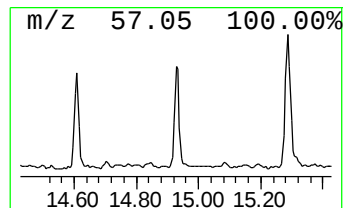
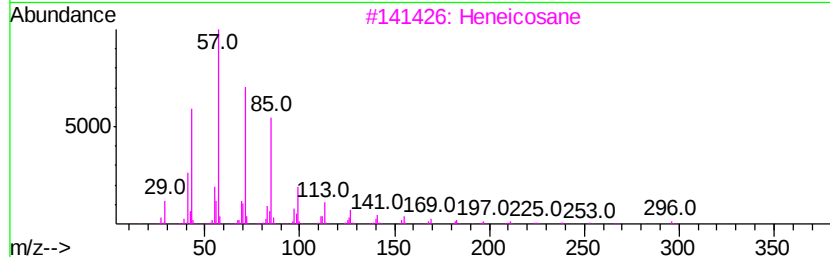
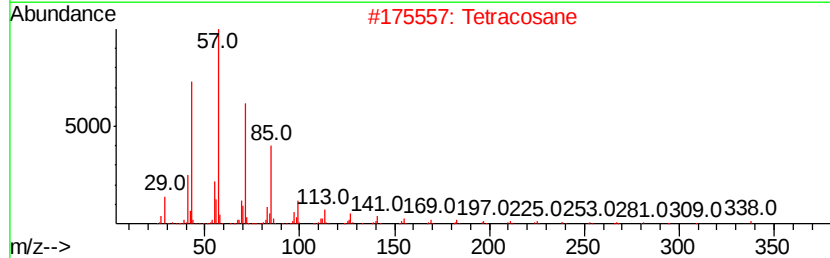
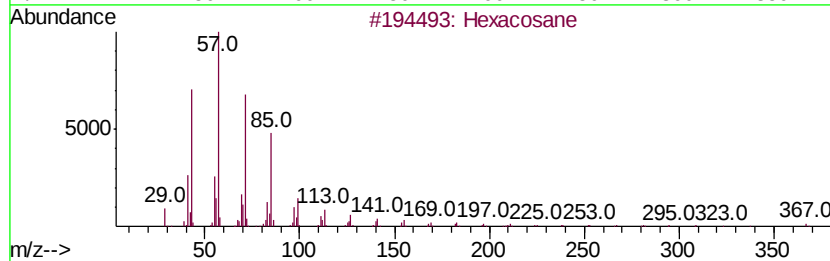
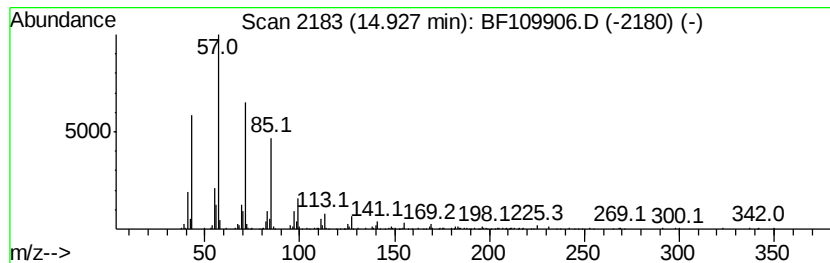
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.60 ng	280309	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Tetracosane	338	C24H50	000646-31-1	90
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane	240	C17H36	000629-78-7	86
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
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Sample : J5526-14
Misc :
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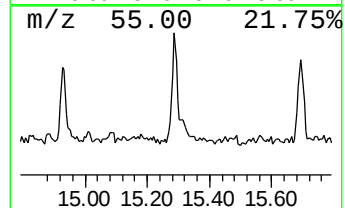
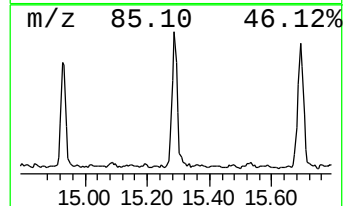
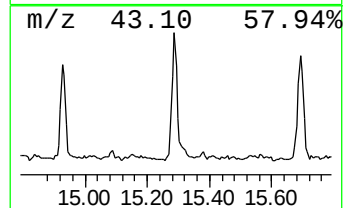
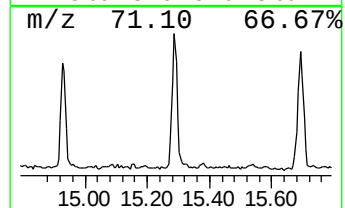
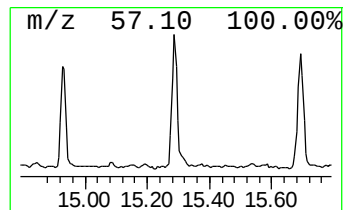
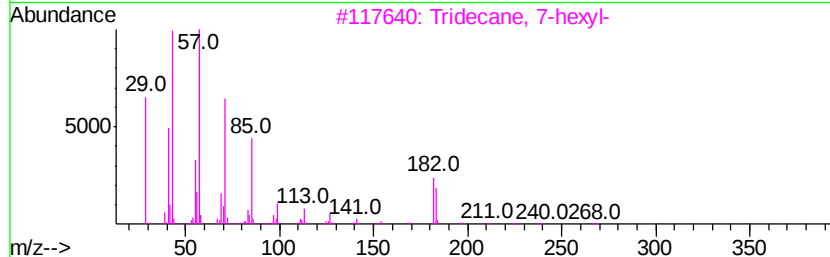
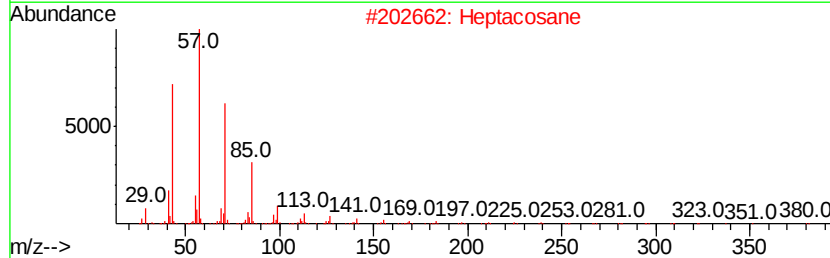
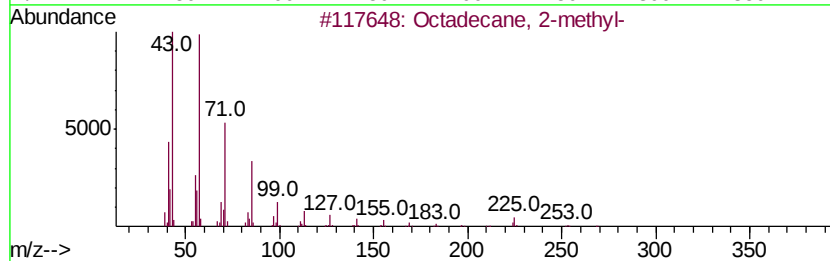
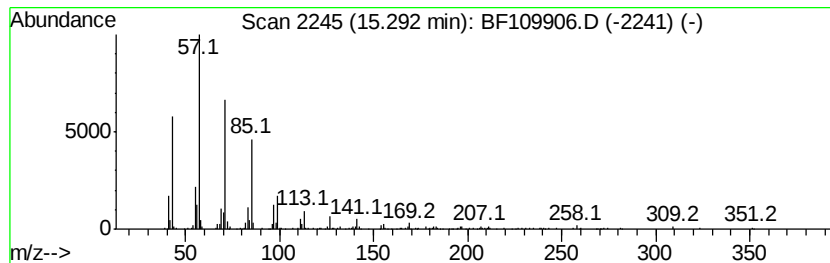
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.29	3.53 ng	379565	Perylene-d12	15.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	94
2	Heptacosane	380	C27H56	000593-49-7	91
3	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
Operator : JU/SJ
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Instrument :
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ClientSampleId :
SUP-4B-C-101518-3

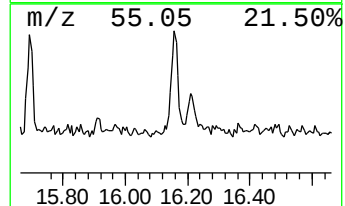
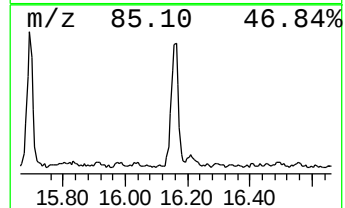
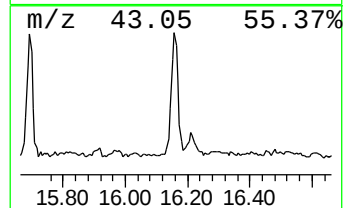
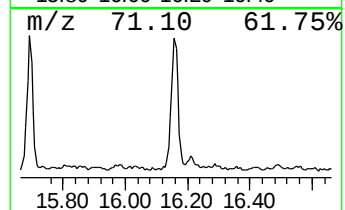
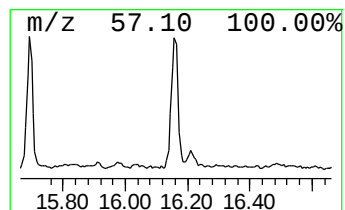
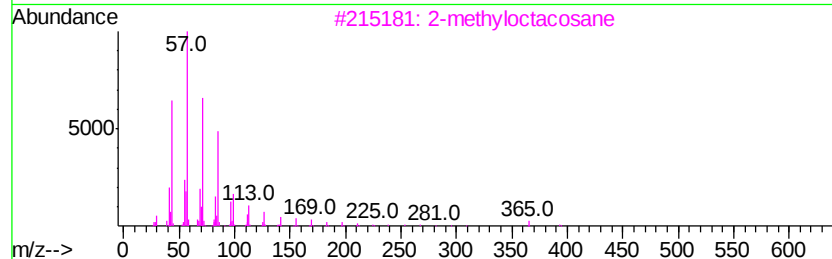
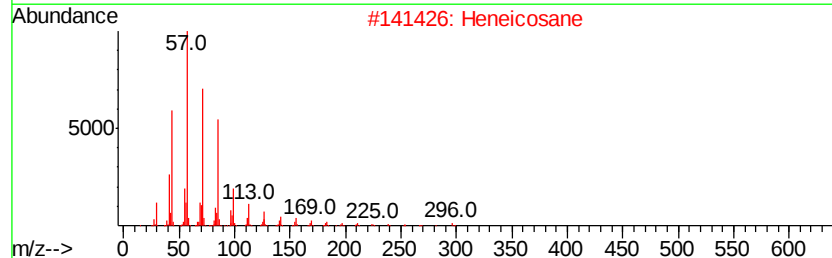
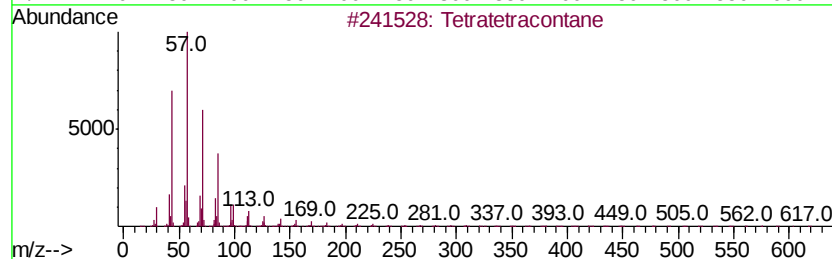
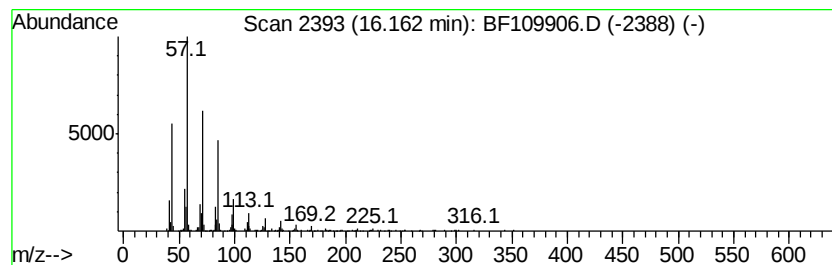
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetratetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	3.49 ng	375506	Perylene-d12	15.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetratetracontane	619	C44H90	007098-22-8	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			2-methyloctacosane	408	C29H60	1000376-72-8	91
4			Octacosane	394	C28H58	000630-02-4	91
5			Hentriacontane	437	C31H64	000630-04-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
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ALS Vial : 8 Sample Multiplier: 1

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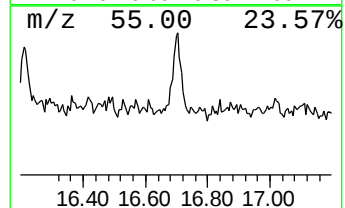
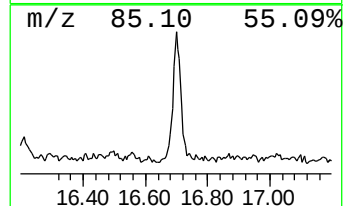
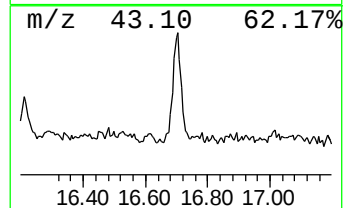
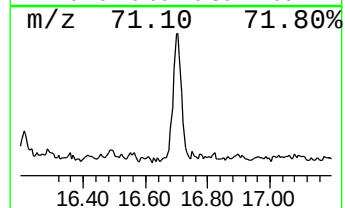
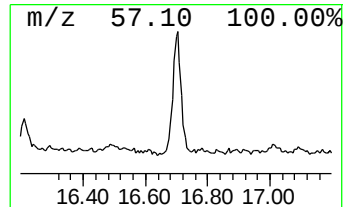
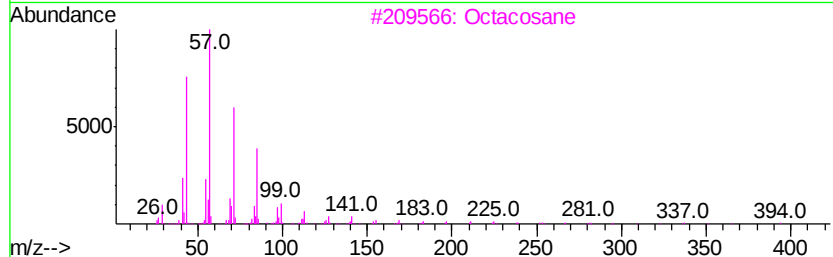
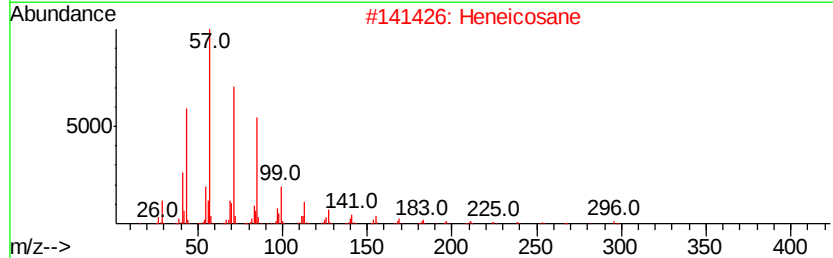
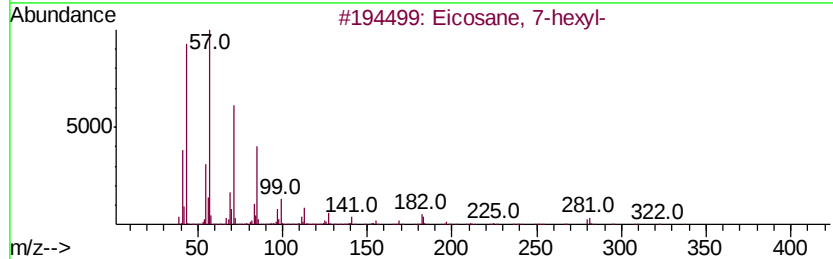
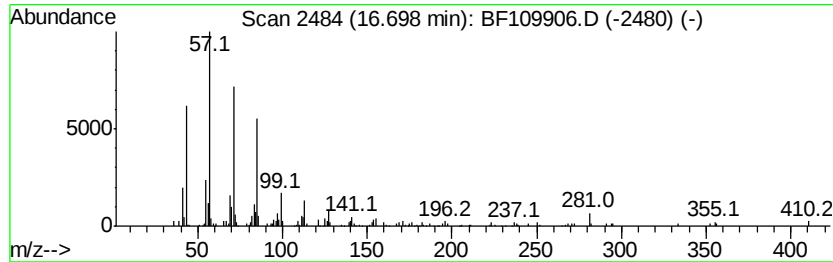
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane, 7-hexyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	2.38 ng	256425	Perylene-d12	15.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
2		Heneicosane	296	C21H44	000629-94-7	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Hexacosane	366	C26H54	000630-01-3	87
5		Hentriacontane	437	C31H64	000630-04-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101618\
Data File : BF109906.D
Acq On : 16 Oct 2018 15:40
Operator : JU/SJ
Sample : J5526-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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(S)-(+)-1,2-Propa...	3.59	2.2	ng	167758	1	6.98	1499180	20.0
2-Pentanone, 4-hy...	5.22	2.8	ng	205972	1	6.98	1499180	20.0
unknown6.75	6.75	65.3	ng	4893490	1	6.98	1499180	20.0
Cyclohexadecane	12.54	2.5	ng	168577	4	11.51	1346160	20.0
1-Docosene	13.97	5.6	ng	533880	5	14.16	1920770	20.0
Hexadecane	14.61	3.1	ng	296075	5	14.16	1920770	20.0
Hexacosane	14.93	2.6	ng	280309	6	15.69	2152680	20.0
Octadecane, 2-met...	15.29	3.5	ng	379565	6	15.69	2152680	20.0
Tetratetracontane	16.16	3.5	ng	375506	6	15.69	2152680	20.0
Eicosane, 7-hexyl-	16.70	2.4	ng	256425	6	15.69	2152680	20.0