

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
 Data File : BF085447.D
 Acq On : 15 Mar 2016 1:08
 Operator : UM/SJ
 Sample : H1730-02
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 W170TH-SB-23-COMP(0.5-1.5)

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-BF030316.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	5.121	246	248	254	rBV	194399	261674	7.00%	0.690%
2	5.521	280	283	286	rBV	2778214	3572361	95.56%	9.413%
3	6.550	370	373	376	rBV	2669084	3738539	100.00%	9.851%
4	6.687	383	385	388	rBV	3113117	3667337	98.10%	9.663%
5	6.927	403	406	408	rBV	737750	989793	26.48%	2.608%
6	7.076	417	419	422	rBV	2620174	2822148	75.49%	7.436%
7	7.487	452	455	457	rBV	2497301	2407550	64.40%	6.344%
8	7.567	460	462	465	rBV	48978	50733	1.36%	0.134%
9	8.207	516	518	520	rBV	1626627	1324330	35.42%	3.490%
10	9.282	610	612	615	rBV	3269052	3570634	95.51%	9.408%
11	9.682	645	647	648	rBV	615895	720282	19.27%	1.898%
12	9.888	663	665	667	rVB	75589	104884	2.81%	0.276%
13	9.968	669	672	674	rVV	1295790	1316881	35.22%	3.470%
14	10.128	683	686	687	rBV	24991	39230	1.05%	0.103%
15	10.162	687	689	692	rVB3	27541	54903	1.47%	0.145%
16	10.390	708	709	711	rVB	210342	165500	4.43%	0.436%
17	10.608	726	728	732	rBV2	58173	115658	3.09%	0.305%
18	10.756	738	741	743	rBV	2035574	2310538	61.80%	6.088%
19	10.870	749	751	757	rBV	135332	252145	6.74%	0.664%
20	11.053	765	767	771	rBV2	24898	49235	1.32%	0.130%
21	11.316	787	790	791	rBV	83441	101370	2.71%	0.267%
22	11.339	791	792	795	rVB	35072	42824	1.15%	0.113%
23	11.453	799	802	805	rBV	844087	1328224	35.53%	3.500%
24	11.522	805	808	810	rVB	72703	83653	2.24%	0.220%
25	11.682	819	822	825	rBV3	14922	41410	1.11%	0.109%
26	11.945	843	845	846	rBV	35498	41318	1.11%	0.109%
27	11.968	846	847	850	rVV2	170542	245165	6.56%	0.646%
28	12.059	853	855	859	rVB2	74608	108647	2.91%	0.286%
29	12.653	905	907	910	rBV	318993	405859	10.86%	1.069%
30	12.756	914	916	919	rBV	88546	100777	2.70%	0.266%
31	12.882	924	927	930	rVV2	266408	383587	10.26%	1.011%
32	13.031	938	940	943	rVB	2531010	2395118	64.07%	6.311%
33	13.111	943	947	950	rBV3	25459	49852	1.33%	0.131%
34	13.214	953	956	958	rBV	64887	76876	2.06%	0.203%

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Integrator: RTE
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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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35	13.316	963	965	969	rVB2	40958	60218	1.61%	0.159%
36	13.602	987	990	994	rBV6	20262	70290	1.88%	0.185%
37	13.831	1007	1010	1012	rBV	36424	69956	1.87%	0.184%
38	13.922	1017	1018	1024	rVB	223311	320237	8.57%	0.844%
39	14.082	1028	1032	1038	rBV2	929098	1279444	34.22%	3.371%
40	14.185	1039	1041	1043	rBV2	27912	43588	1.17%	0.115%
41	14.471	1064	1066	1067	rBV	38709	37712	1.01%	0.099%
42	14.562	1071	1074	1075	rBV3	52984	76801	2.05%	0.202%
43	14.837	1096	1098	1101	rBV2	114532	160858	4.30%	0.424%
44	14.928	1104	1106	1110	rVB	85715	128402	3.43%	0.338%
45	15.122	1120	1123	1127	rBV	179942	387351	10.36%	1.021%
46	15.191	1127	1129	1131	rBV	164493	191330	5.12%	0.504%
47	15.419	1146	1149	1152	rVB	110835	166786	4.46%	0.439%
48	15.477	1152	1154	1157	rBV	162903	222605	5.95%	0.587%
49	15.545	1157	1160	1165	rVB	588560	882208	23.60%	2.325%
50	16.002	1197	1200	1203	rBV	125760	213908	5.72%	0.564%
51	16.060	1203	1205	1207	rVV2	44546	73944	1.98%	0.195%
52	16.242	1219	1221	1226	rVB2	93686	206730	5.53%	0.545%
53	16.665	1256	1258	1264	rVB2	66534	155285	4.15%	0.409%
54	16.985	1283	1286	1292	rVB2	65868	146890	3.93%	0.387%
55	17.420	1321	1324	1330	rBV	50312	117653	3.15%	0.310%

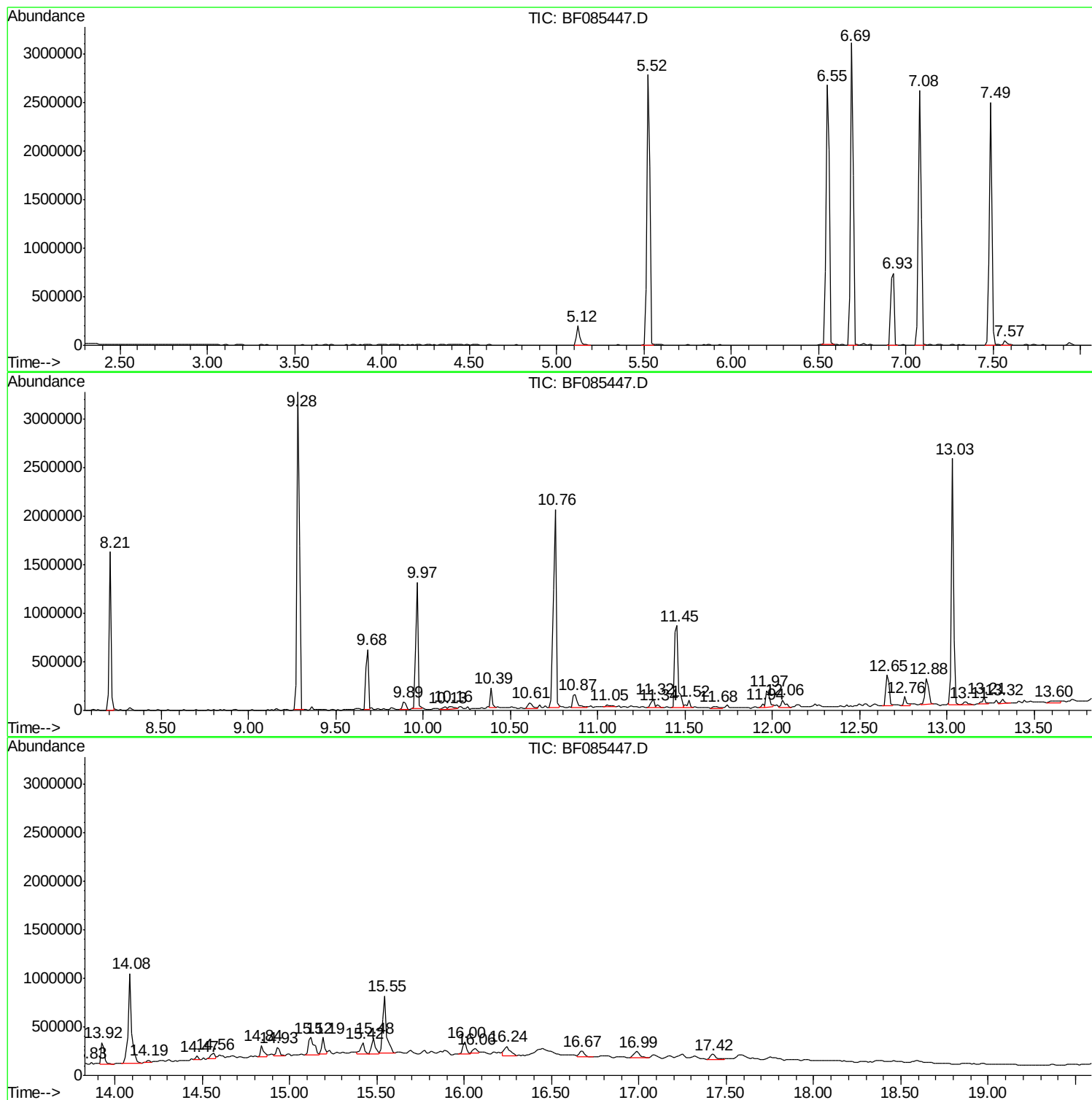
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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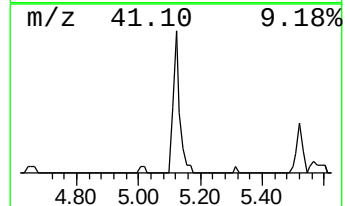
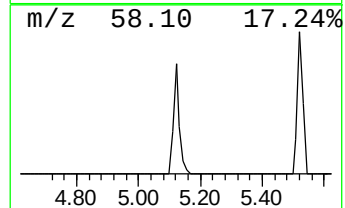
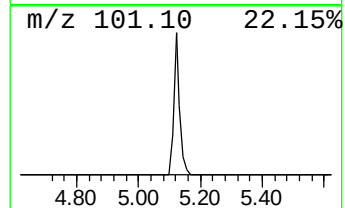
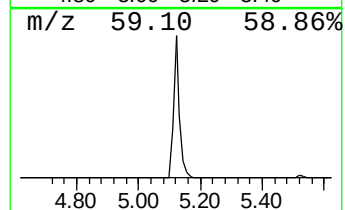
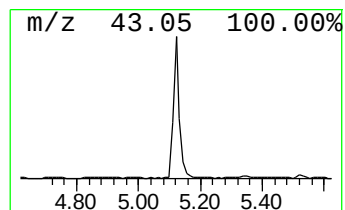
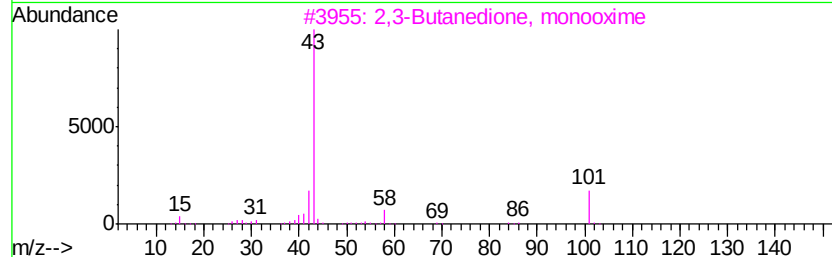
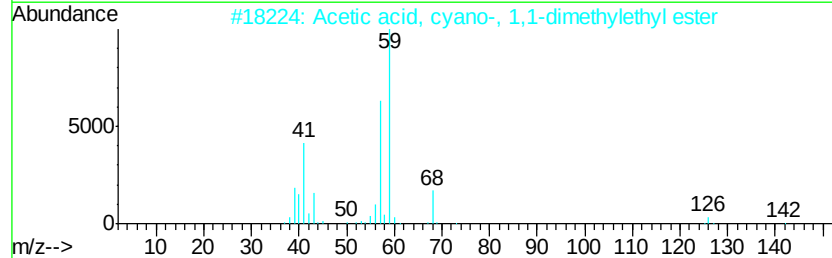
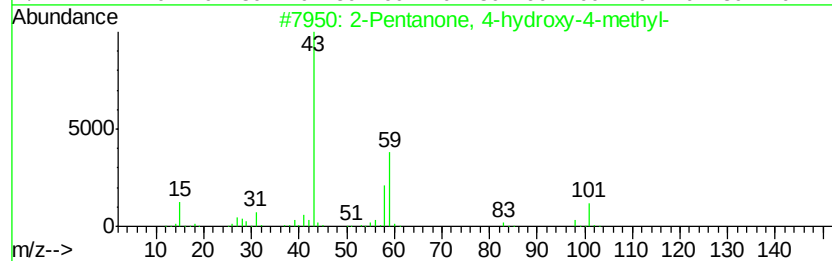
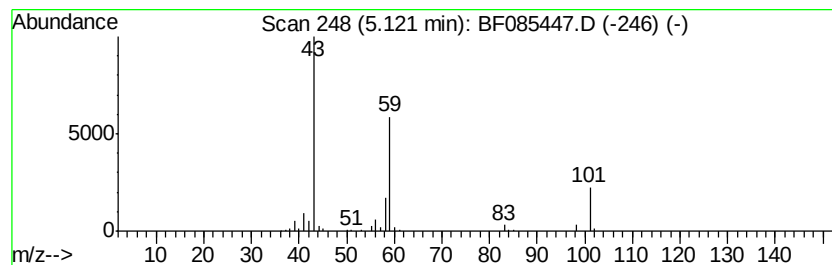
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	5.29 ng	261674	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4			Acetone	58	C3H6O	000067-64-1	10
5			Butane	58	C4H10	000106-97-8	9



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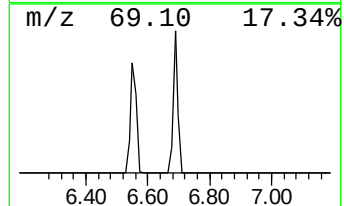
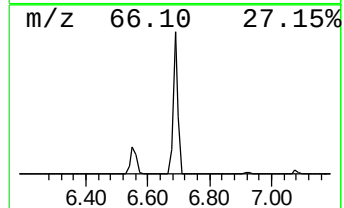
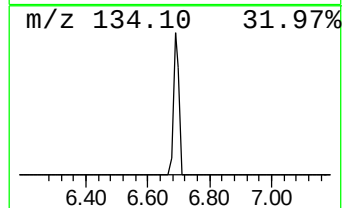
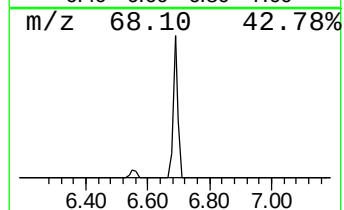
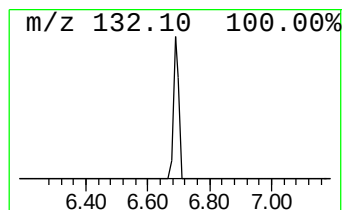
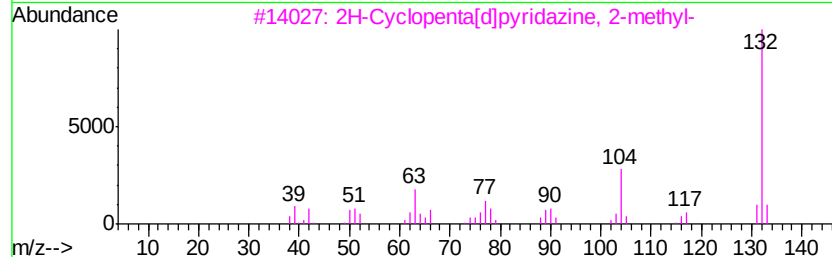
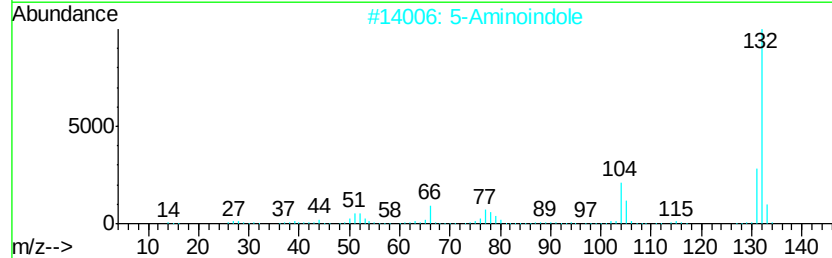
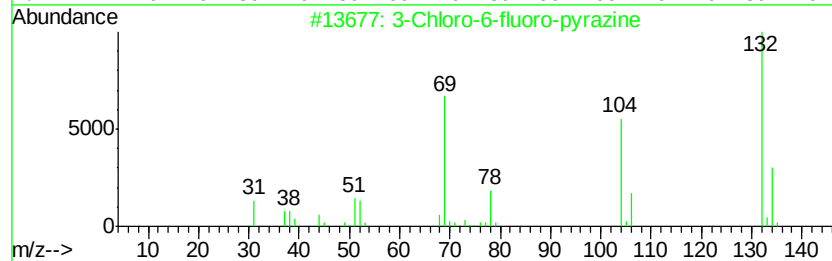
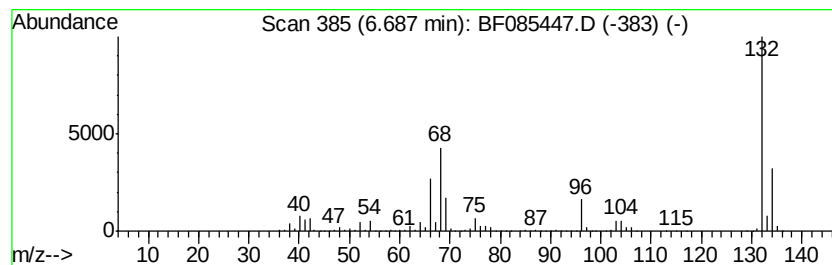
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	74.10 ng	3667340	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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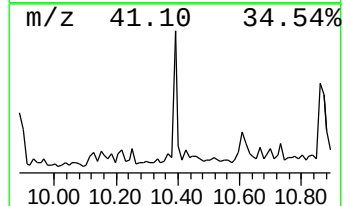
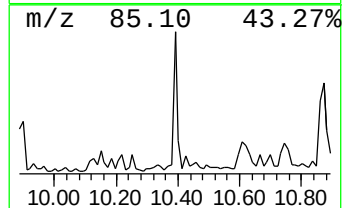
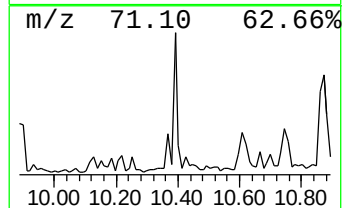
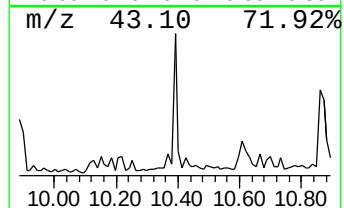
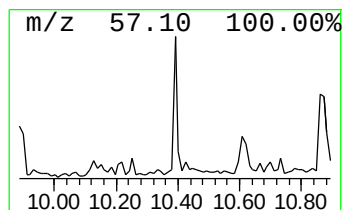
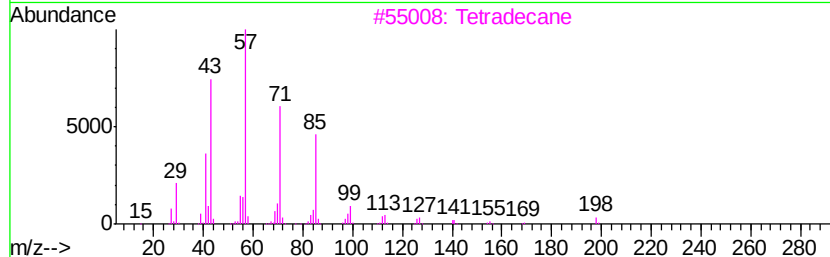
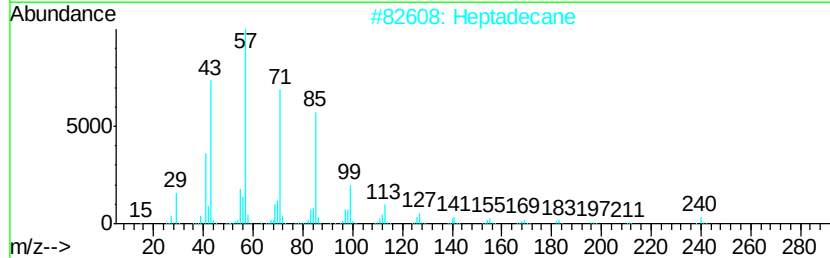
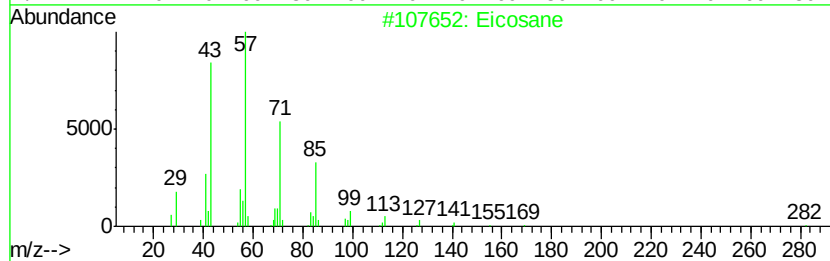
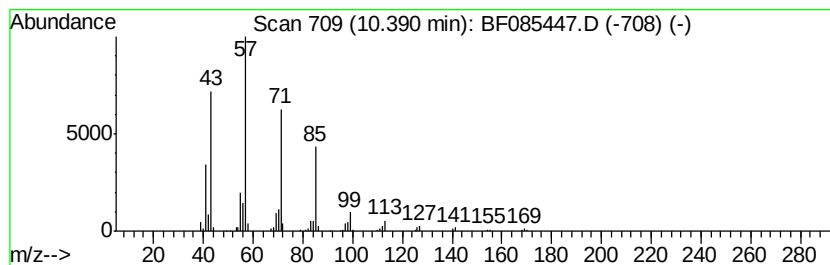
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	2.51 ng	165500	Acenaphthene-d10	9.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	91
2		Heptadecane	240	C17H36	000629-78-7	90
3		Tetradecane	198	C14H30	000629-59-4	86
4		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	80



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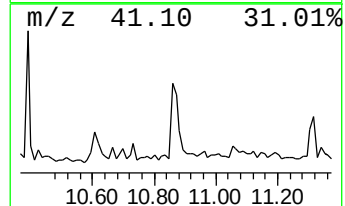
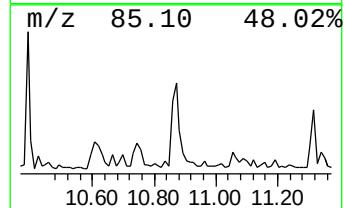
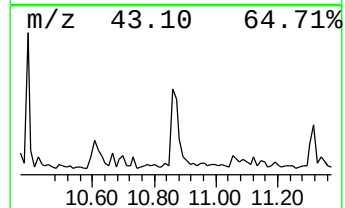
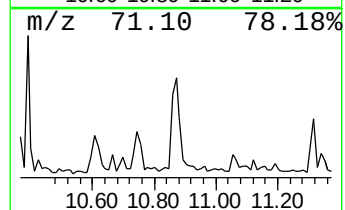
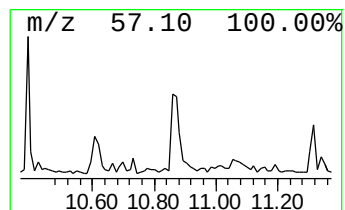
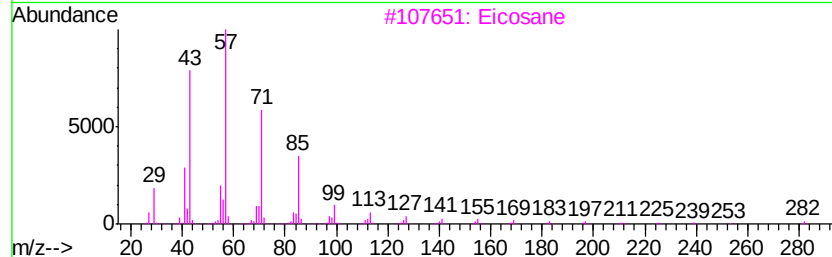
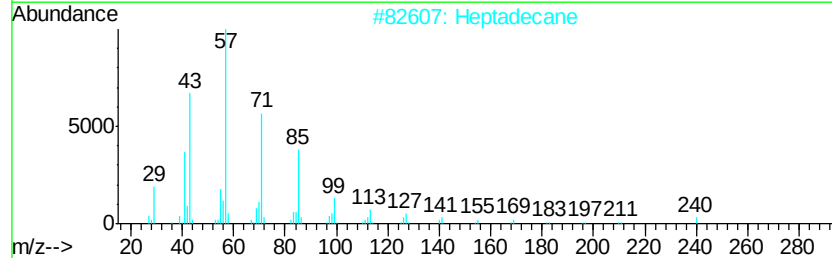
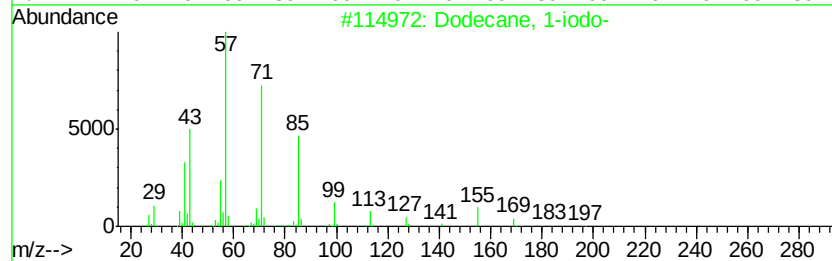
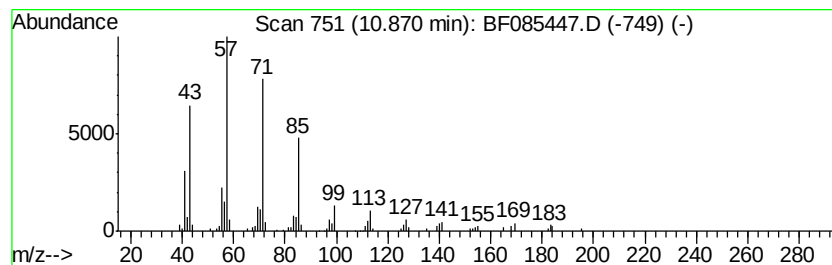
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 1-iodo- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.87	3.80 ng	252145	Phenanthrene-d10	11.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Tridecane	184	C13H28	000629-50-5	90
5	Tetratetracontane	619	C44H90	007098-22-8	90



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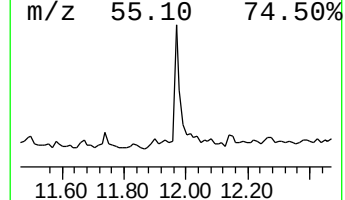
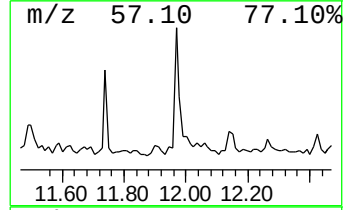
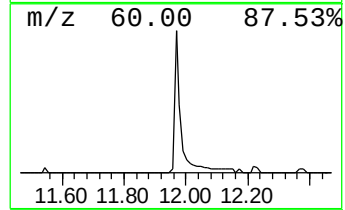
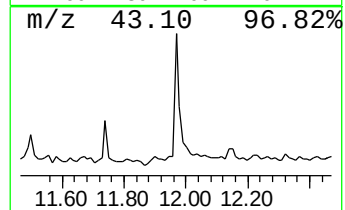
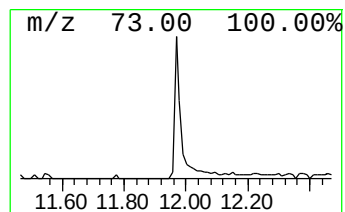
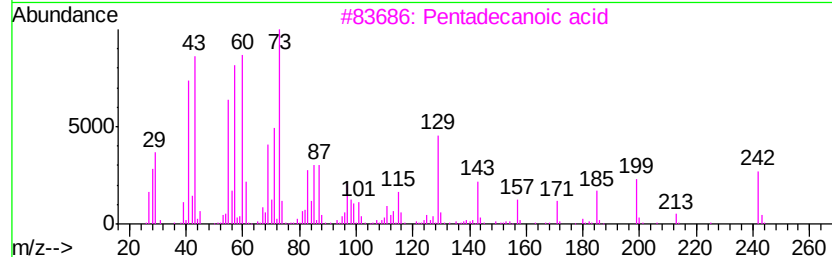
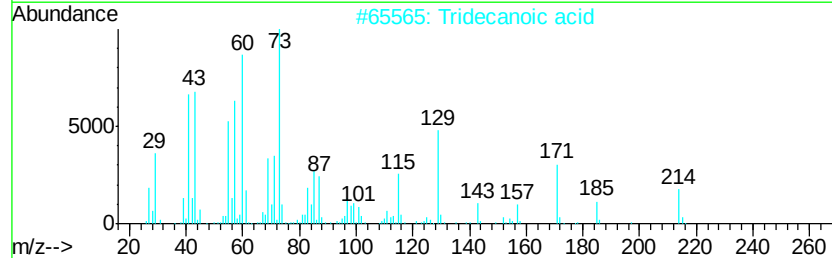
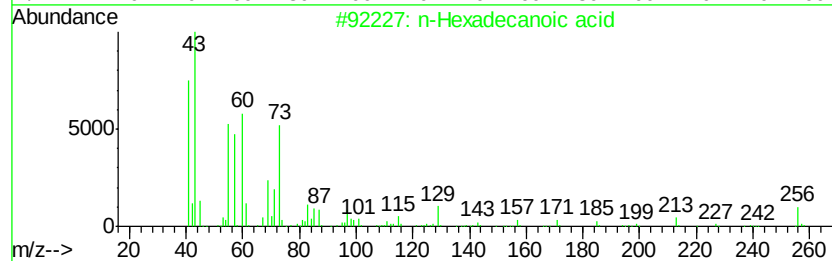
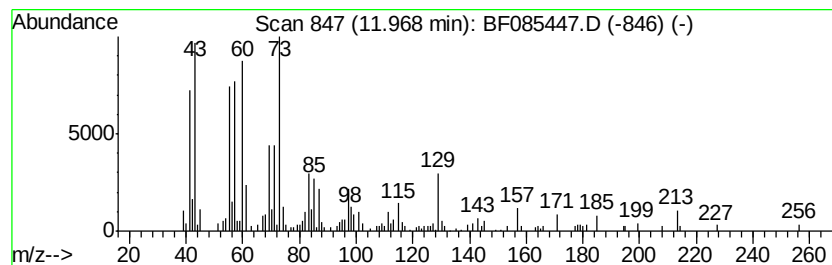
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	3.69 ng	245165	Phenanthrene-d10	11.45

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Nonanoic acid	158	C9H18O2	000112-05-0	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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Acq On : 15 Mar 2016 1:08
Operator : UM/SJ
Sample : H1730-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

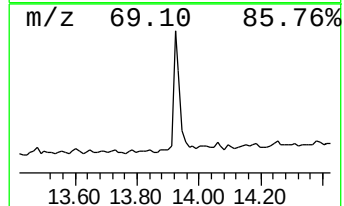
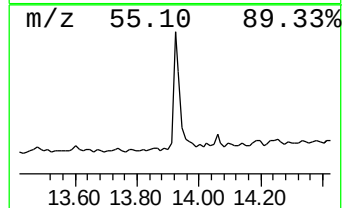
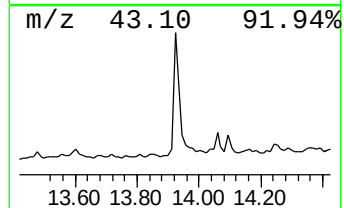
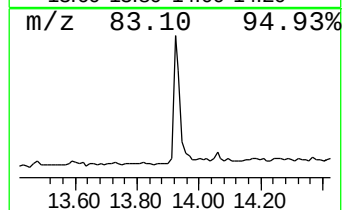
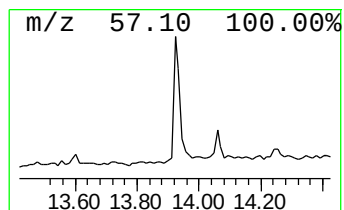
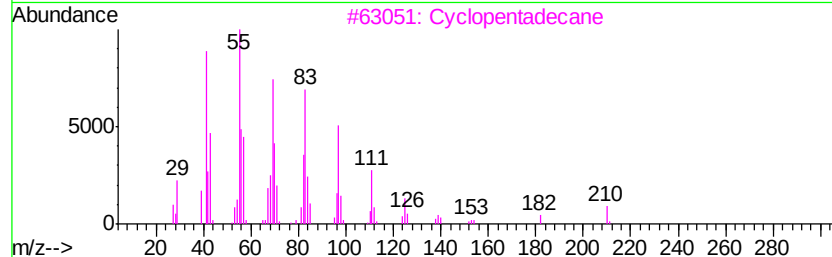
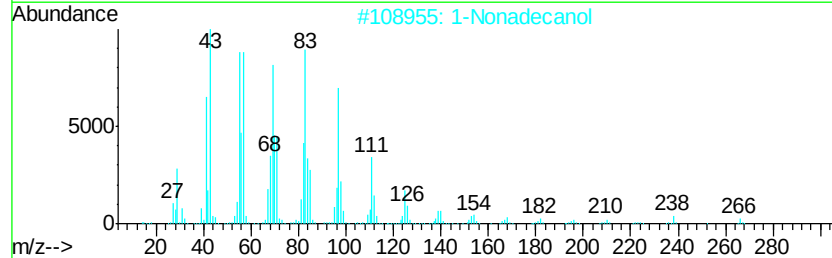
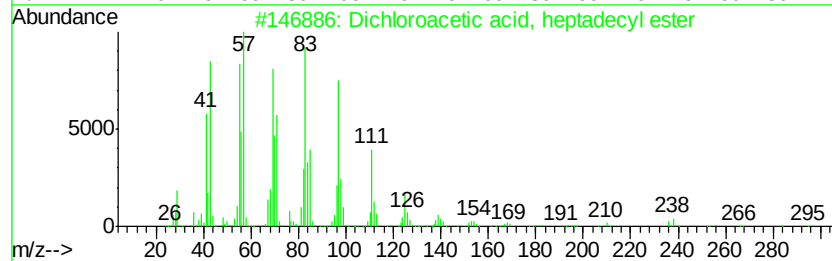
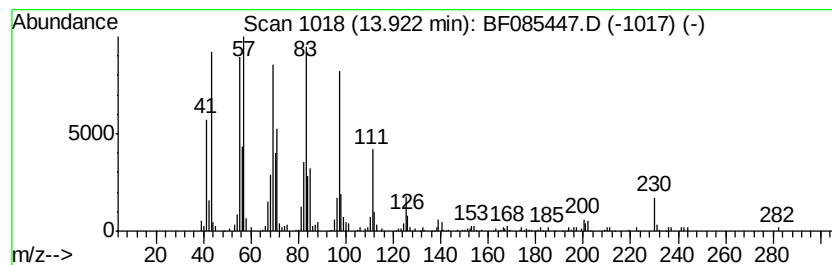
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.92	5.01 ng	320237	Chrysene-d12	14.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	1-Nonadecanol	284	C19H40O	001454-84-8	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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Sample : H1730-02
Misc :
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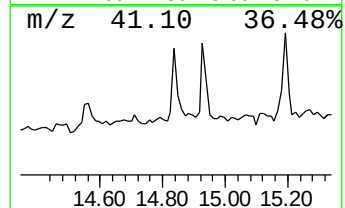
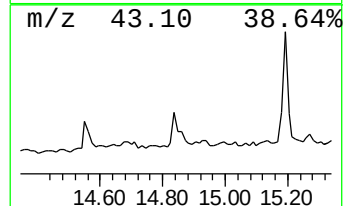
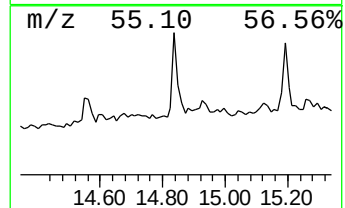
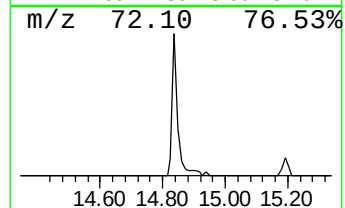
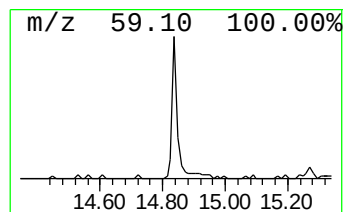
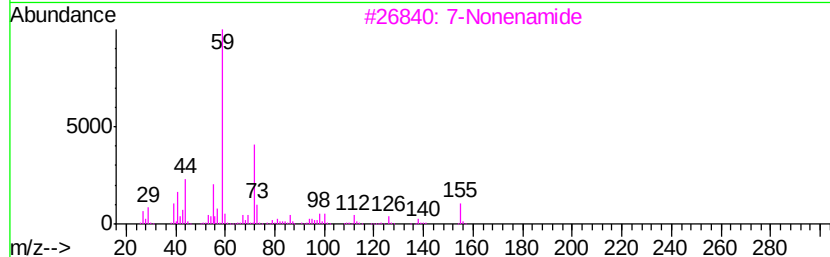
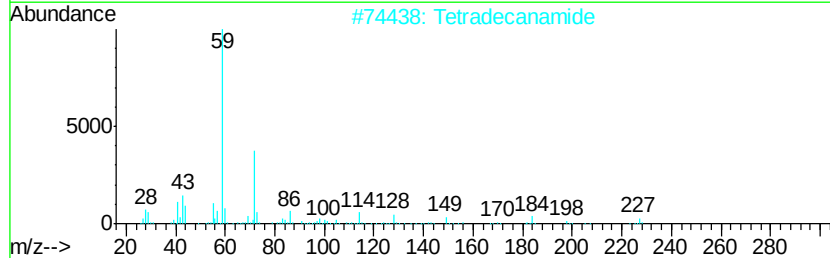
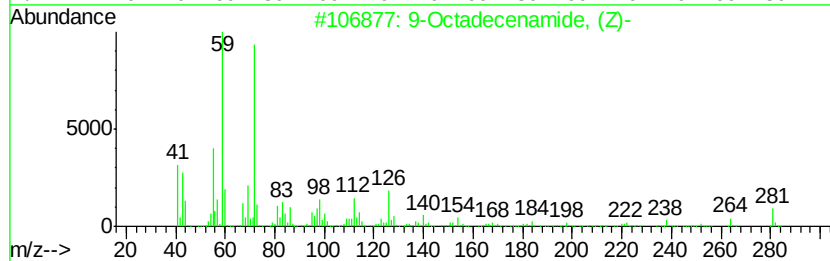
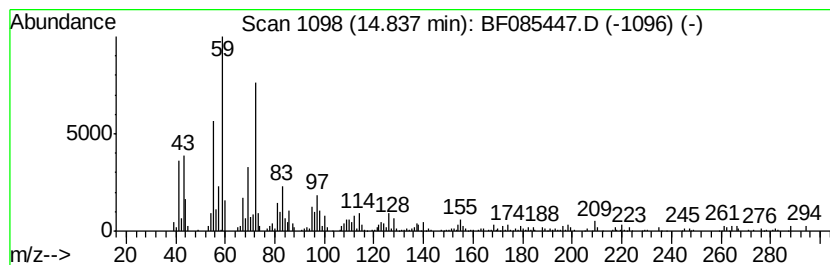
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.84	3.65 ng	160858	Perylene-d12	15.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	56
2	Tetradecanamide	227	C14H29NO	000638-58-4	53
3	7-Nonenamide	155	C9H17NO	090949-53-4	47
4	Dodecanamide	199	C12H25NO	001120-16-7	43
5	1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	41



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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Sample : H1730-02
Misc :
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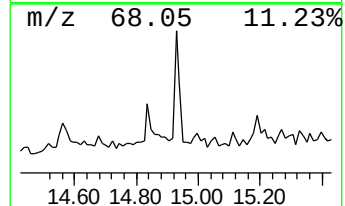
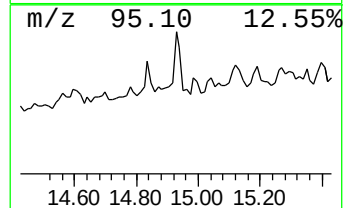
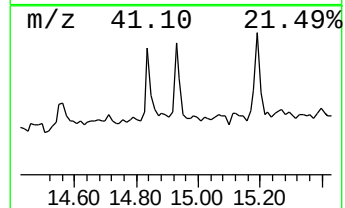
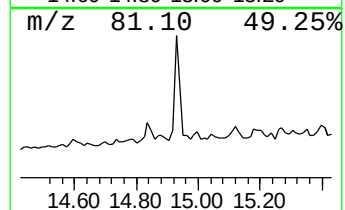
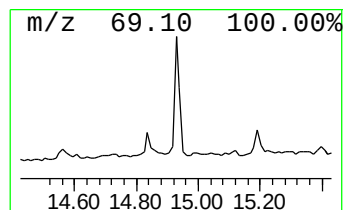
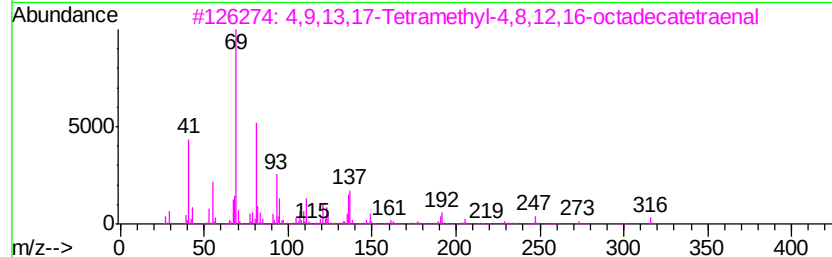
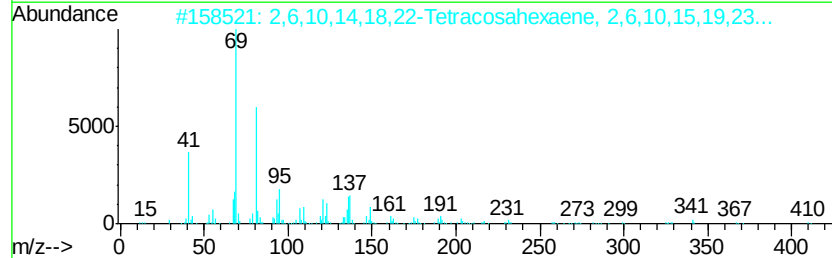
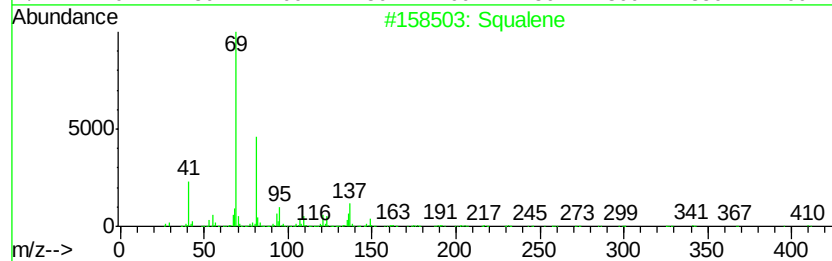
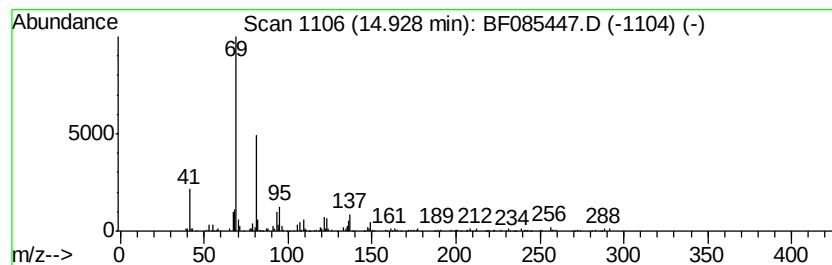
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	2.91 ng	128402	Perylene-d12	15.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	90
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	86
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	64
4	2,3,5-Trimethyl-2,3,5-hexanetric...	203 C12H17N3	003974-79-6	64
5	5,9,13-Pentadecatrien-2-one, 6,1...	262 C18H30O	001117-52-8	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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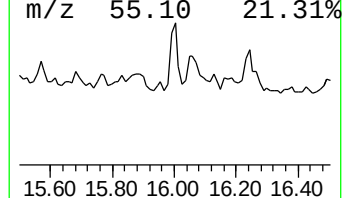
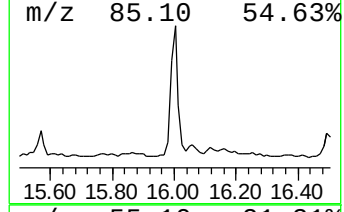
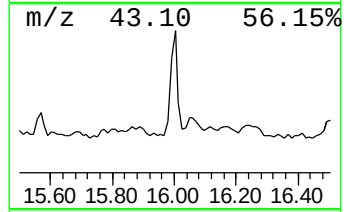
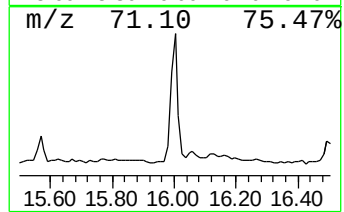
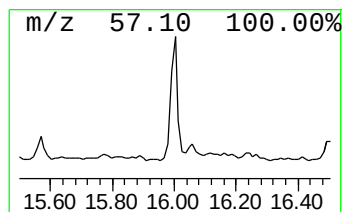
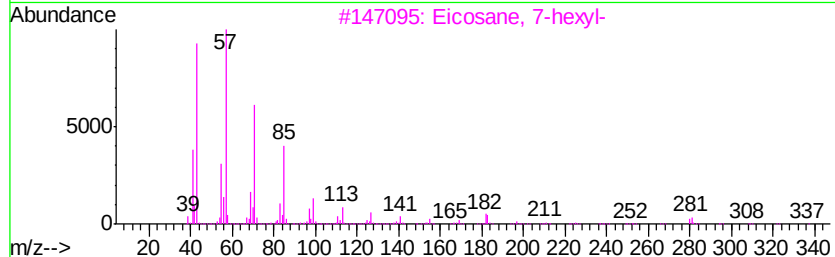
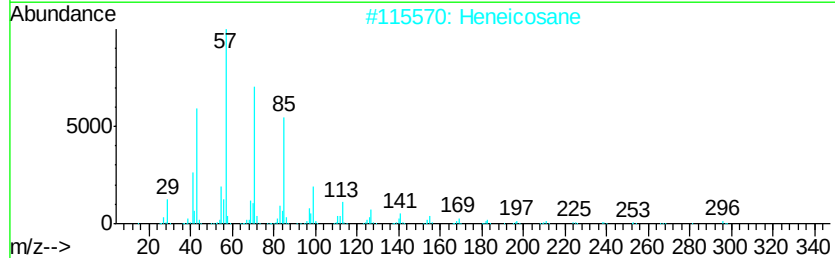
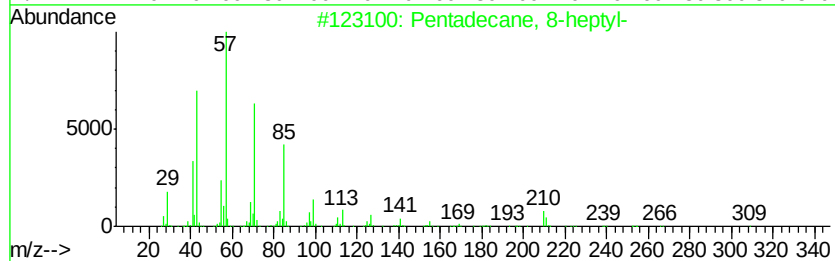
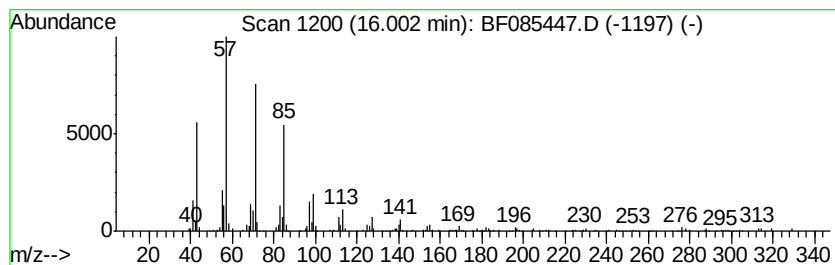
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentadecane, 8-heptyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.00	4.85 ng	213908	Perylene-d12	15.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	90
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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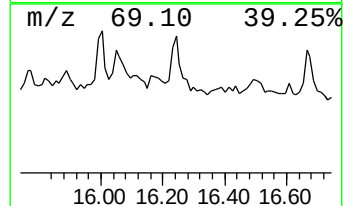
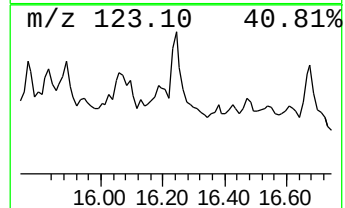
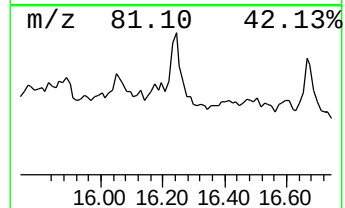
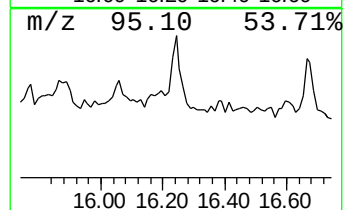
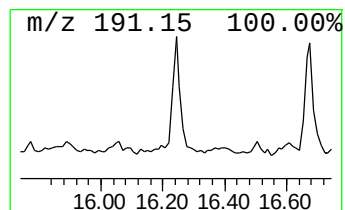
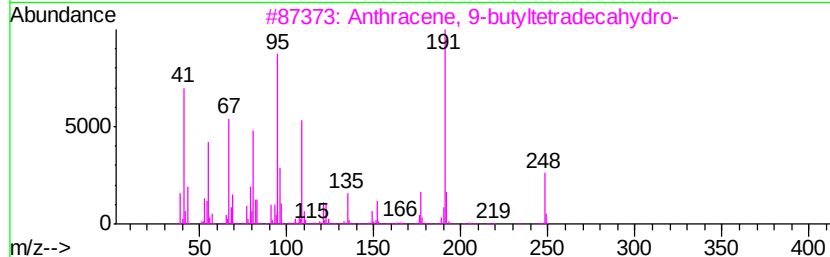
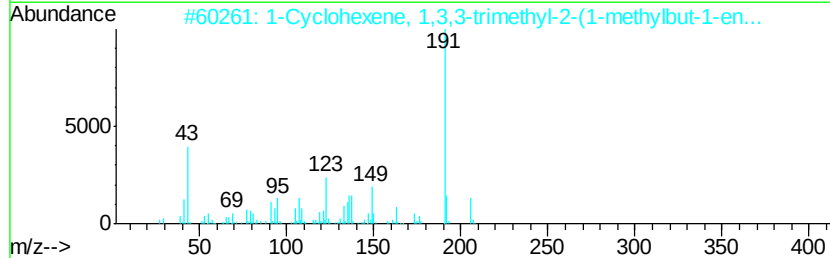
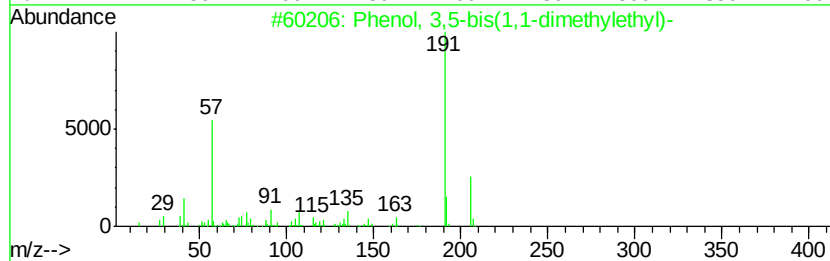
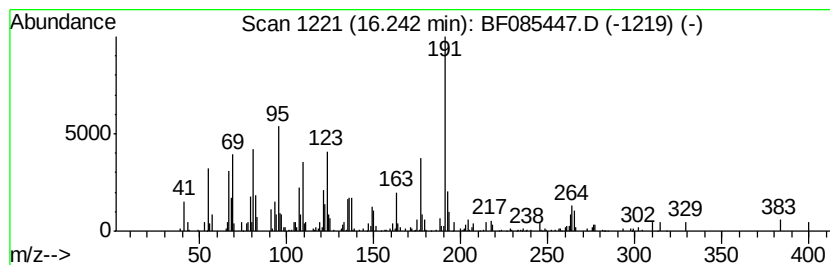
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown16.24 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	4.69 ng	206730	Perylene-d12	15.55
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 3,5-bis(1,1-dimethylethyl)-	206 C14H22O	001138-52-9	35
2	1-Cyclohexene, 1,3,3-trimethyl-2...	206 C14H22O	1000197-08-4	32
3	Anthracene, 9-butyldodecahydro-	248 C18H32	055133-89-6	32
4	Anthracene, 9-cyclohexyldodec...	274 C20H34	055255-70-4	27
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206 C14H22O	005875-45-6	27



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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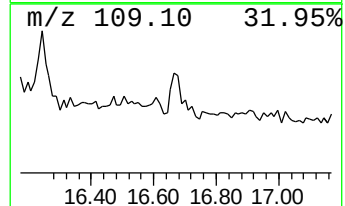
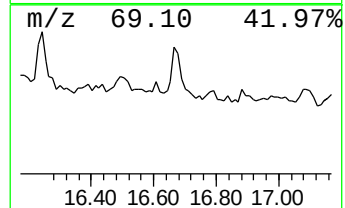
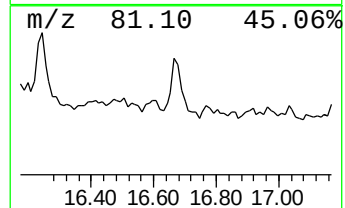
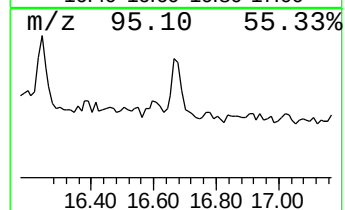
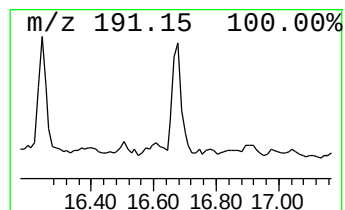
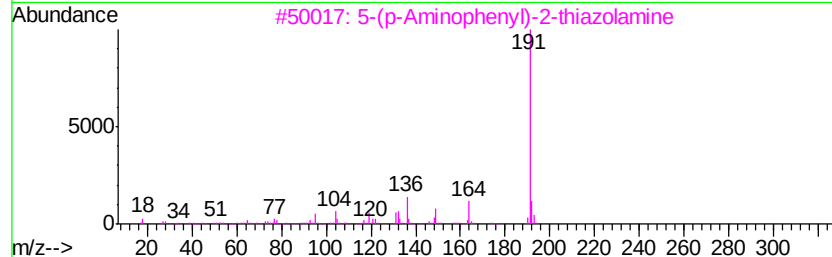
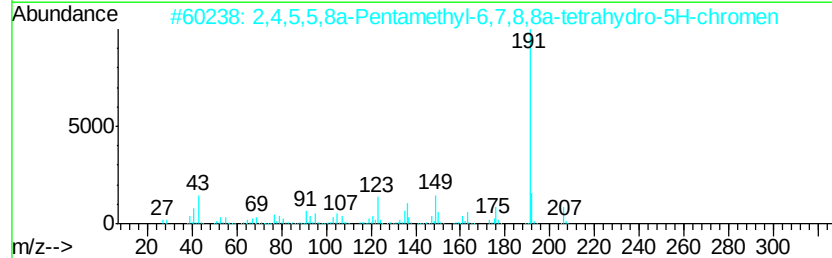
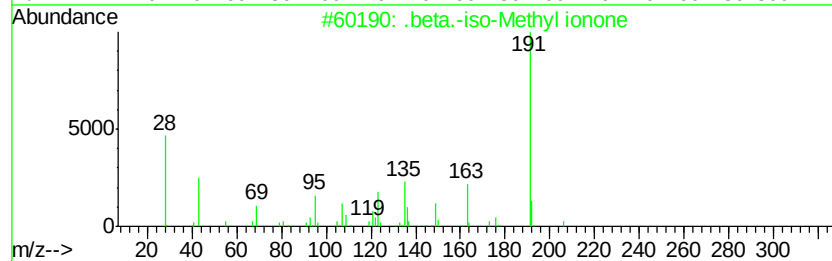
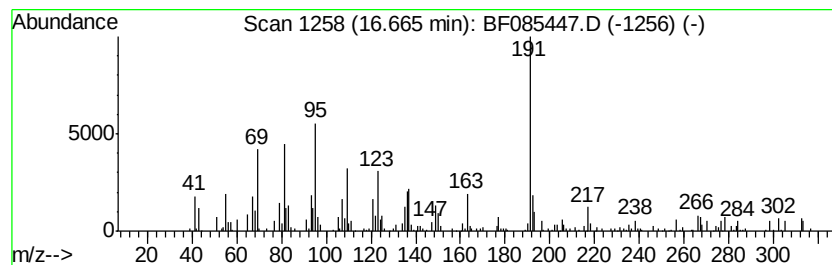
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .beta.-iso-Methyl ionone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.67	3.52 ng	155285	Perylene-d12	15.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	81
2	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	47
3	5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	46
4	Cyclopropene, 3-bromo-1,2-diphenyl-	270	C15H11Br	029559-17-9	43
5	Anthracene, 9-cyclohexyltetradec...	274	C20H34	055255-70-4	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
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Acq On : 15 Mar 2016 1:08
Operator : UM/SJ
Sample : H1730-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
W170TH-SB-23-COMP(0.5-1.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.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...	5.12	5.3	ng	261674	1	6.93	989793	20.0
unknown6.69	6.69	74.1	ng	3667340	1	6.93	989793	20.0
Eicosane	10.39	2.5	ng	165500	3	9.97	1316880	20.0
Dodecane, 1-iodo-	10.87	3.8	ng	252145	4	11.45	1328220	20.0
n-Hexadecanoic acid	11.97	3.7	ng	245165	4	11.45	1328220	20.0
Dichloroacetic ac...	13.92	5.0	ng	320237	5	14.08	1279440	20.0
9-Octadecenamide,...	14.84	3.6	ng	160858	6	15.55	882208	20.0
Squalene	14.93	2.9	ng	128402	6	15.55	882208	20.0
Pentadecane, 8-he...	16.00	4.8	ng	213908	6	15.55	882208	20.0
unknown16.24	16.24	4.7	ng	206730	6	15.55	882208	20.0
.beta.-iso-Methyl...	16.67	3.5	ng	155285	6	15.55	882208	20.0