

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111289.D
 Acq On : 11 Dec 2018 21:14
 Operator : JU/SJ
 Sample : J6157-07
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-4-TOTAL

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-BF120818.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	2.834	120	127	134	rVB	242505	389311	8.55%	0.924%
2	3.799	286	291	302	rBV2	32646	57177	1.26%	0.136%
3	4.040	327	332	336	rBV	56461	71904	1.58%	0.171%
4	4.363	382	387	396	rBV	382767	445981	9.80%	1.058%
5	4.987	487	493	504	rVB	868086	897638	19.72%	2.130%
6	5.263	536	540	544	rBV	224454	198019	4.35%	0.470%
7	5.404	560	564	575	rBV	1560548	1384073	30.41%	3.284%
8	5.740	618	621	626	rBV	63483	58060	1.28%	0.138%
9	5.922	648	652	655	rBV	71849	64200	1.41%	0.152%
10	6.434	733	739	749	rBV2	1443999	2073264	45.55%	4.919%
11	6.563	757	761	764	rBV	2770366	2389253	52.50%	5.668%
12	6.793	797	800	804	rBV	2079381	1793031	39.40%	4.254%
13	6.863	809	812	819	rBV	81709	82128	1.80%	0.195%
14	6.951	823	827	830	rBV	3939467	3097189	68.05%	7.348%
15	7.351	890	895	898	rBV	3091574	2703601	59.40%	6.414%
16	7.575	930	933	936	rVB	91937	72655	1.60%	0.172%
17	8.075	1014	1018	1022	rBV	2818930	2446630	53.76%	5.804%
18	8.387	1068	1071	1077	rBV	47762	48318	1.06%	0.115%
19	9.157	1197	1202	1205	rBV	4923247	4551137	100.00%	10.797%
20	9.545	1264	1268	1272	rBV	1343535	1048130	23.03%	2.487%
21	9.734	1295	1300	1304	rBV3	29876	55091	1.21%	0.131%
22	9.834	1310	1317	1321	rBV	3188762	2752806	60.49%	6.531%
23	10.034	1348	1351	1355	rBV	70705	65991	1.45%	0.157%
24	10.245	1384	1387	1390	rBV	89589	87548	1.92%	0.208%
25	10.616	1446	1450	1453	rBV	2295608	1926975	42.34%	4.572%
26	11.316	1565	1569	1572	rBV	3264583	2743691	60.29%	6.509%
27	11.710	1633	1636	1641	rVB3	85195	82906	1.82%	0.197%
28	11.775	1644	1647	1650	rBV4	47620	60243	1.32%	0.143%
29	11.857	1655	1661	1676	rBV	3026978	3269437	71.84%	7.756%
30	12.557	1778	1780	1788	rVB2	51796	61178	1.34%	0.145%
31	12.639	1788	1794	1807	rBV	1125995	1110276	24.40%	2.634%
32	12.904	1834	1839	1842	rBV	2601257	2235299	49.12%	5.303%
33	13.810	1989	1993	2006	rBV	354847	493663	10.85%	1.171%
34	13.951	2013	2017	2021	rBV	1502028	1333671	29.30%	3.164%

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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	14.133	2045	2048	2054	rVB	52358	53434	1.17%	0.127%
36	14.439	2097	2100	2106	rBV2	95910	113148	2.49%	0.268%
37	14.745	2148	2152	2156	rVB	120004	132159	2.90%	0.314%
38	14.816	2161	2164	2168	rVB	64339	73938	1.62%	0.175%
39	15.074	2204	2208	2211	rBV	137610	145152	3.19%	0.344%
40	15.392	2257	2262	2267	rBV2	826641	1024889	22.52%	2.431%
41	15.445	2267	2271	2276	rVB	127946	158028	3.47%	0.375%
42	15.868	2339	2343	2347	rBV	95976	136151	2.99%	0.323%
43	15.927	2350	2353	2360	rVB8	33313	66899	1.47%	0.159%
44	16.363	2422	2427	2432	rVB2	57319	97141	2.13%	0.230%

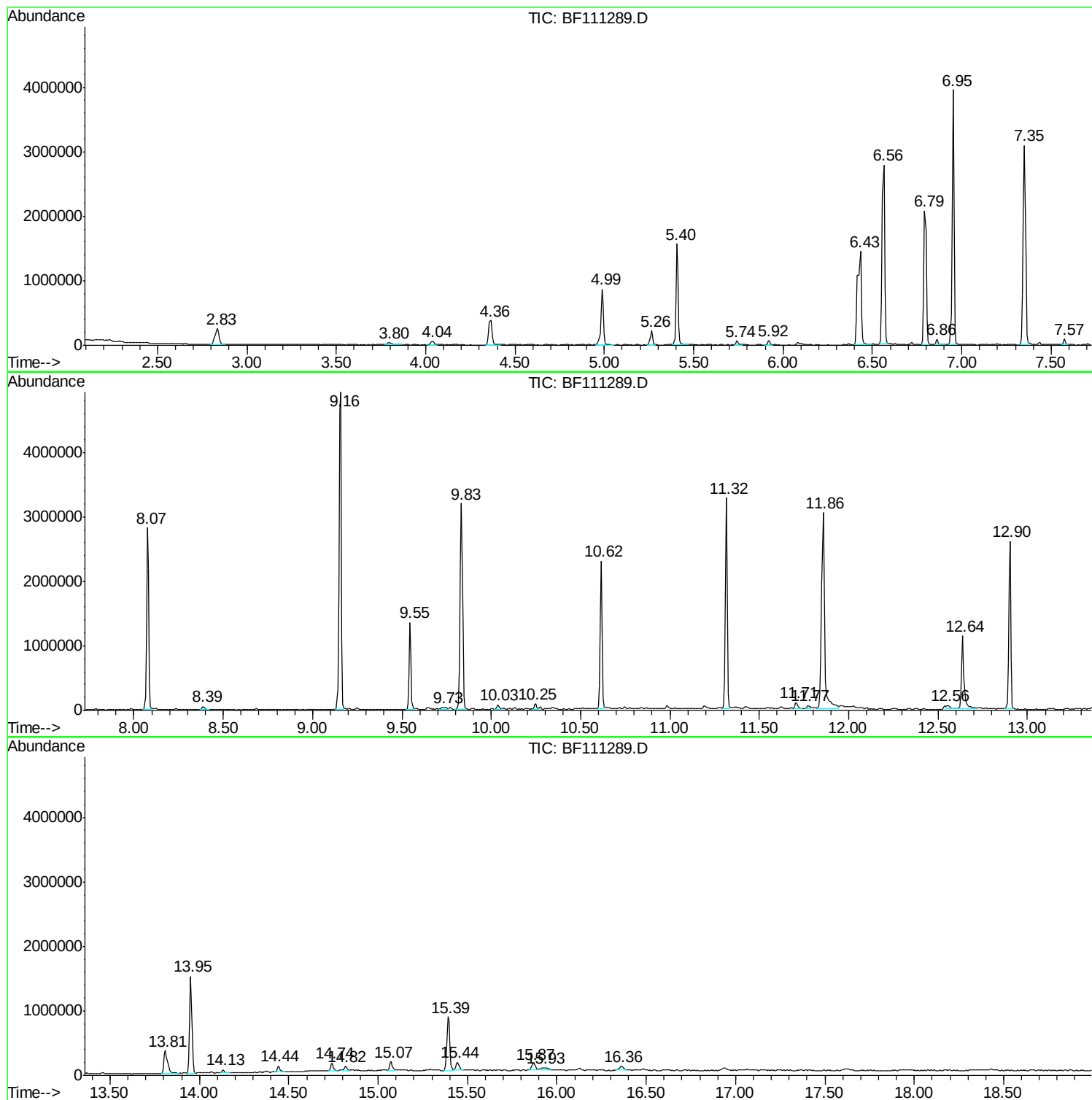
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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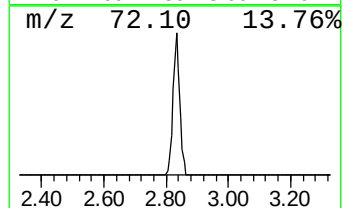
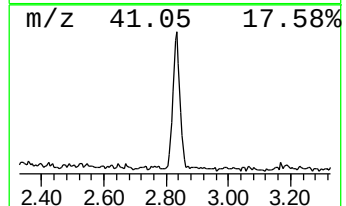
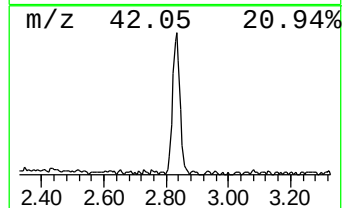
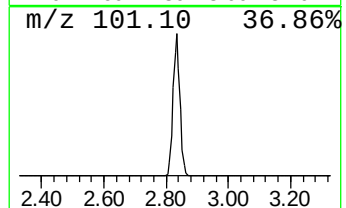
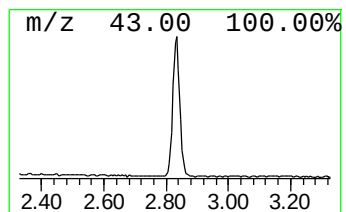
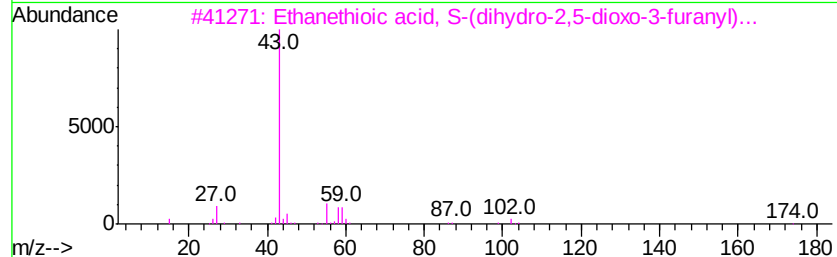
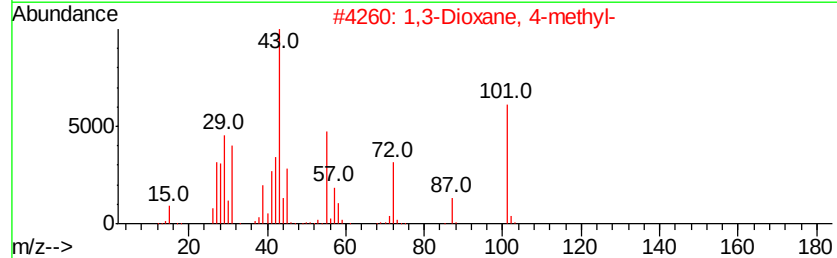
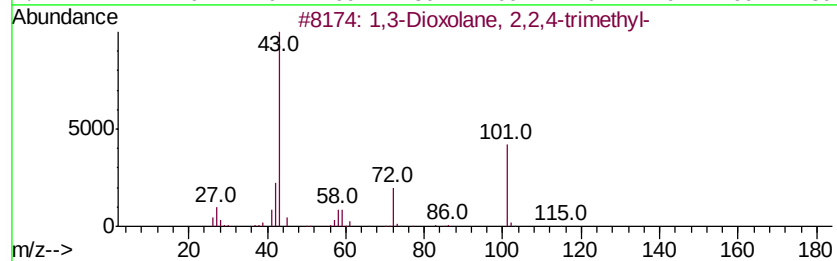
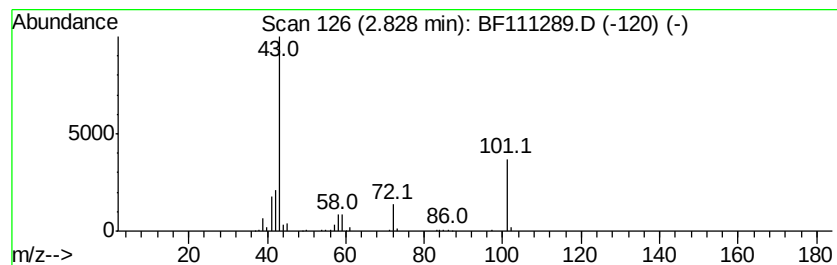
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	4.34 ng	389311	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	64
3		Ethanethioic acid, S-(dihydro-2,5-dioxo-3-furanyl)-	174	C6H6O4S	006953-60-2	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-furan	101	C4H7NO2	016504-58-8	9
5		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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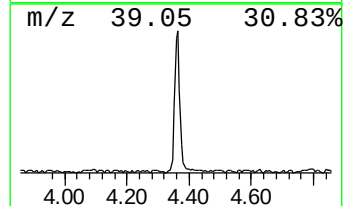
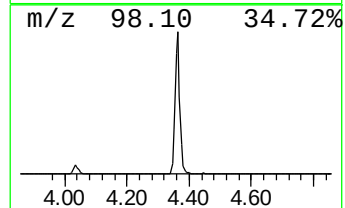
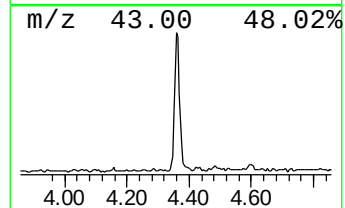
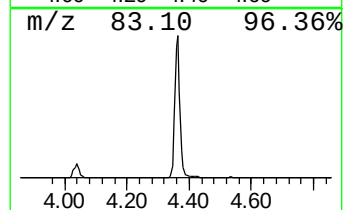
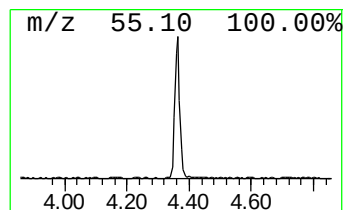
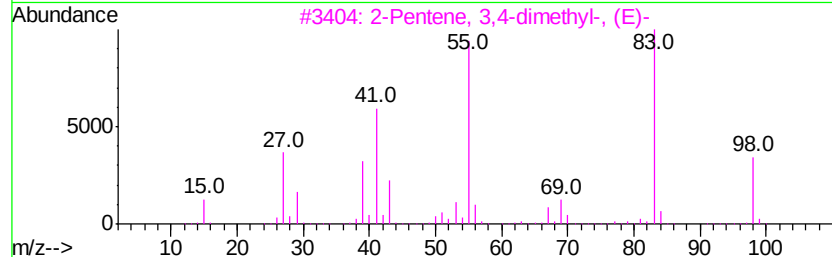
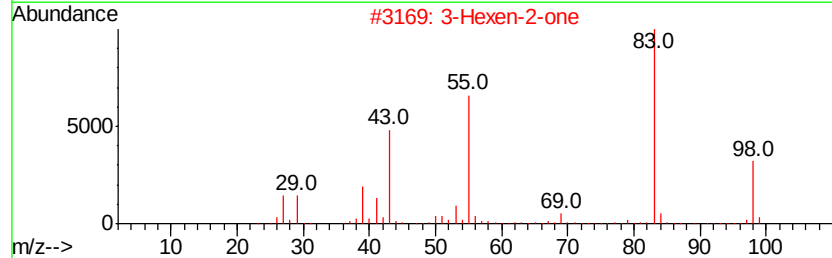
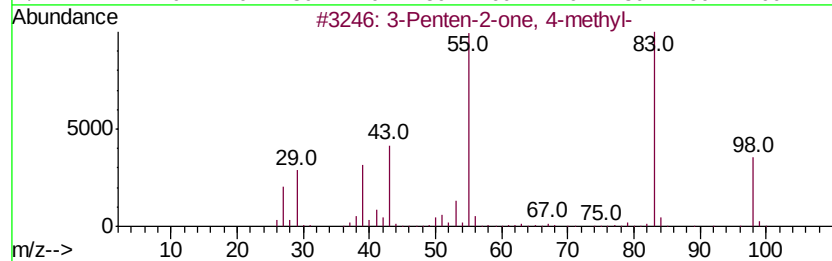
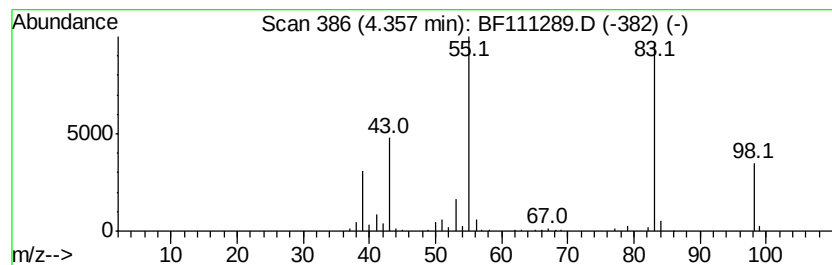
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	4.97 ng	445981	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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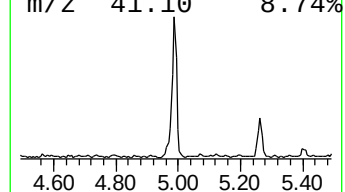
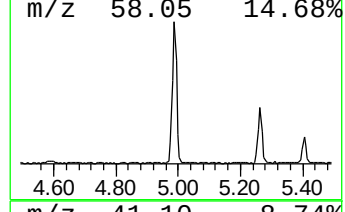
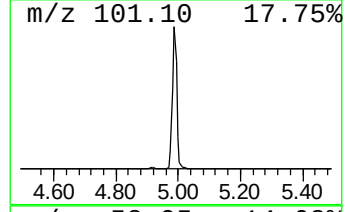
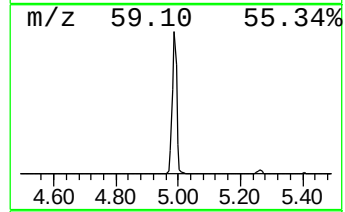
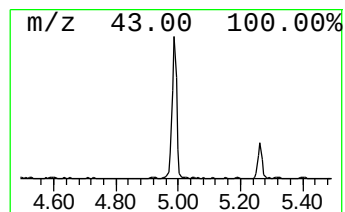
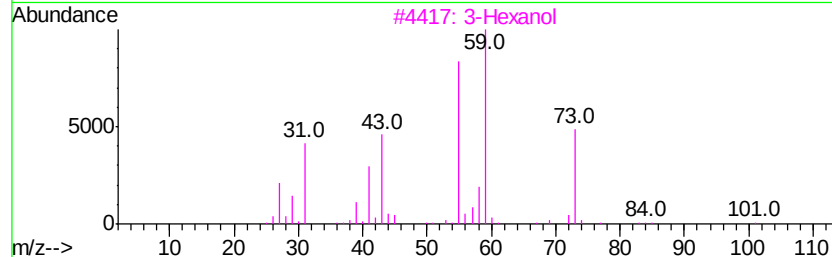
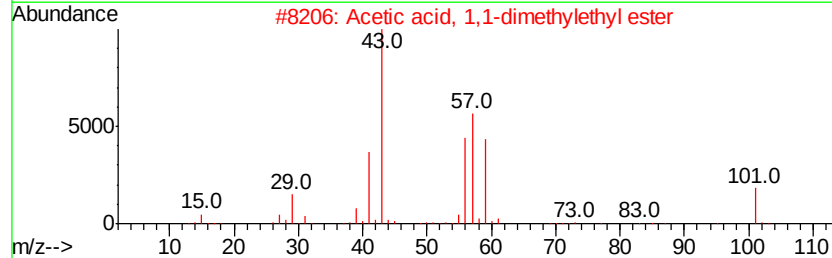
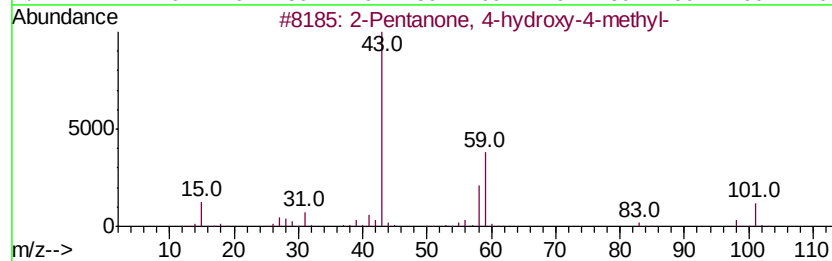
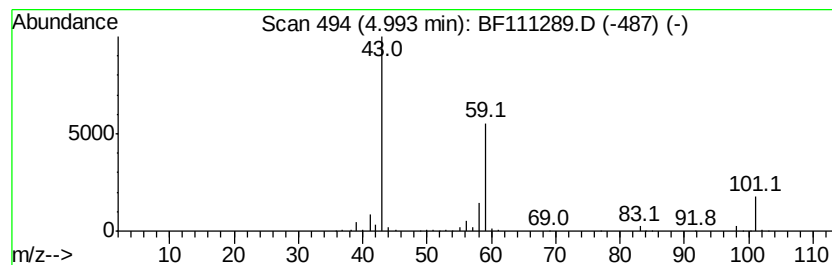
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	10.01 ng	897638	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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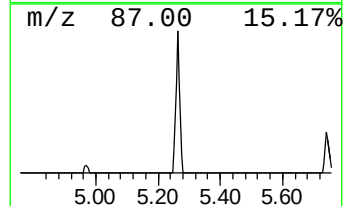
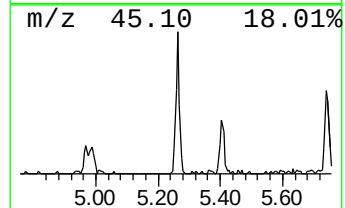
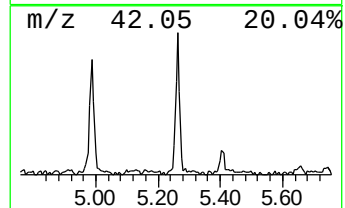
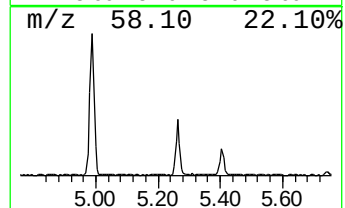
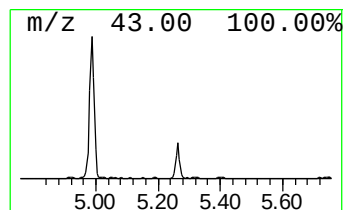
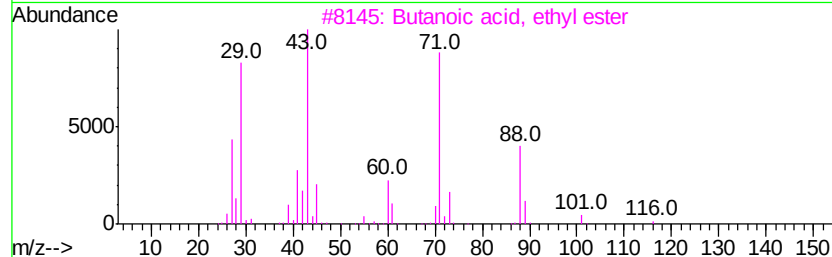
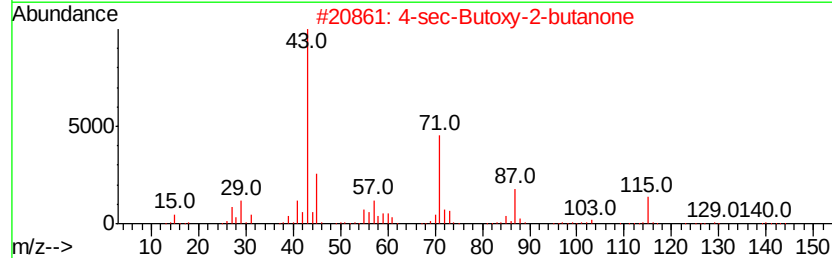
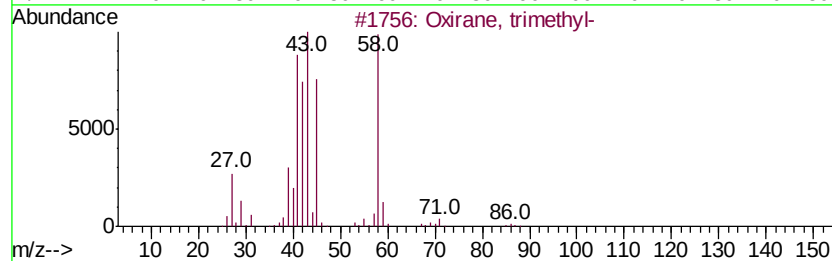
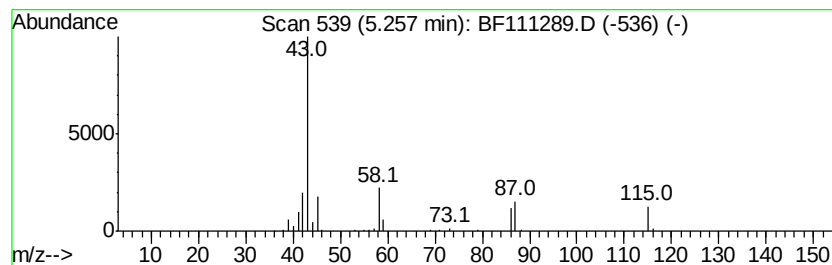
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown5.26 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	2.21 ng	198019	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	28
2		4-sec-Butoxy-2-butanone	144	C8H16O2	057545-63-8	25
3		Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	9
4		2,3-Butanedione	86	C4H6O2	000431-03-8	9
5		Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9



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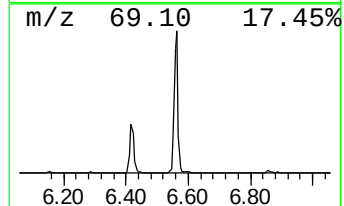
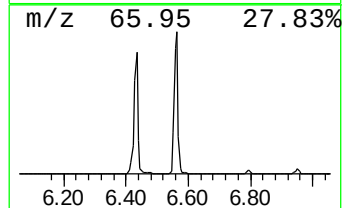
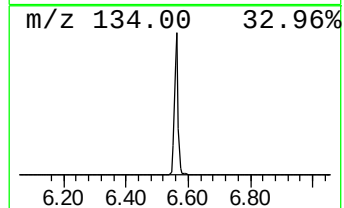
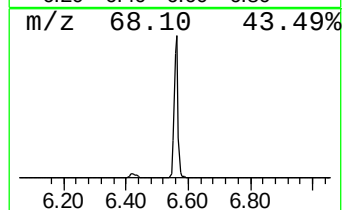
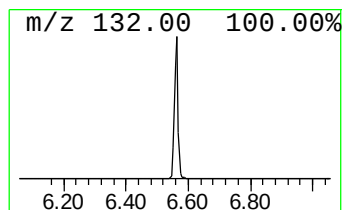
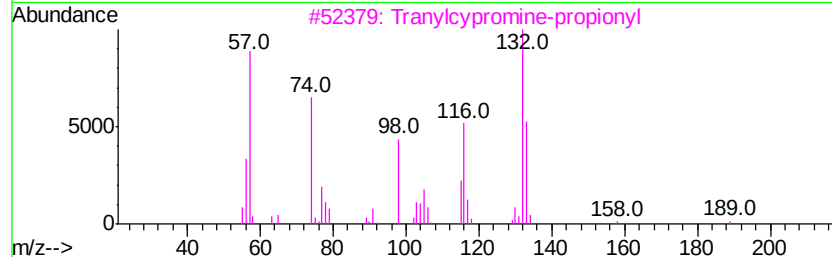
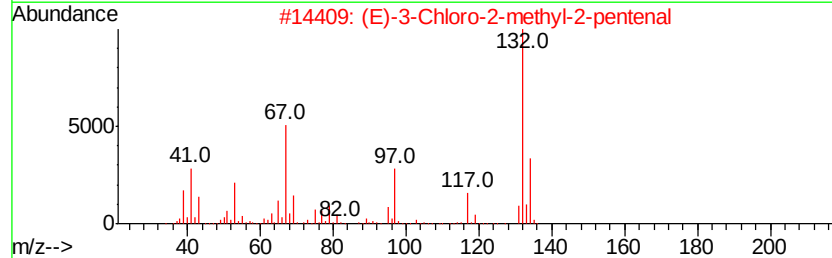
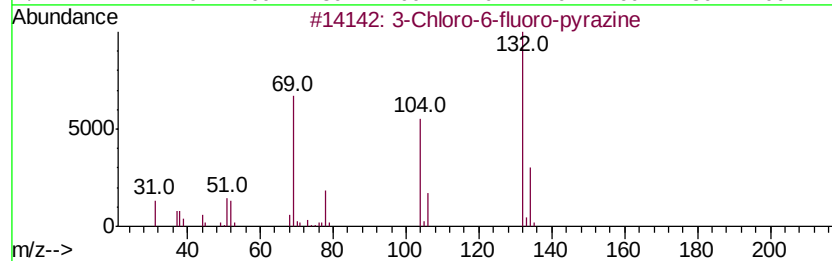
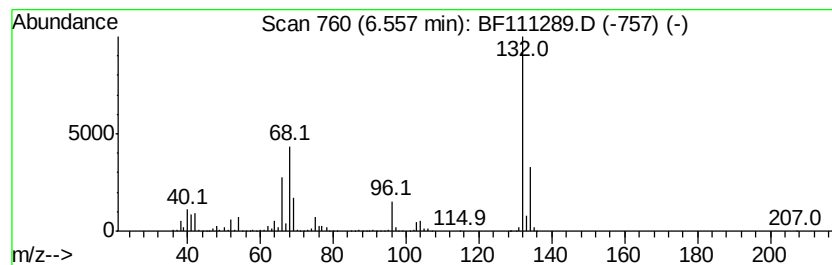
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	26.65 ng	2389250	1,4-Dichlorobenzene-d4	6.79

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	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Xenon	132	Xe	007440-63-3	9



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Data File : BF111289.D
Acq On : 11 Dec 2018 21:14
Operator : JU/SJ
Sample : J6157-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

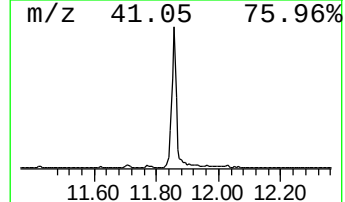
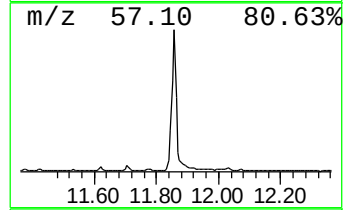
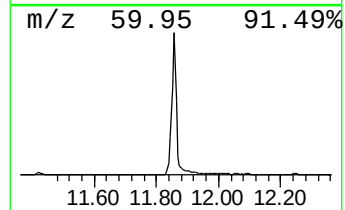
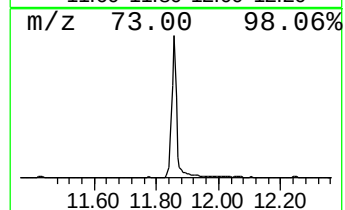
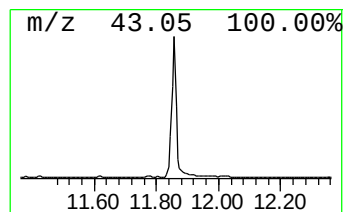
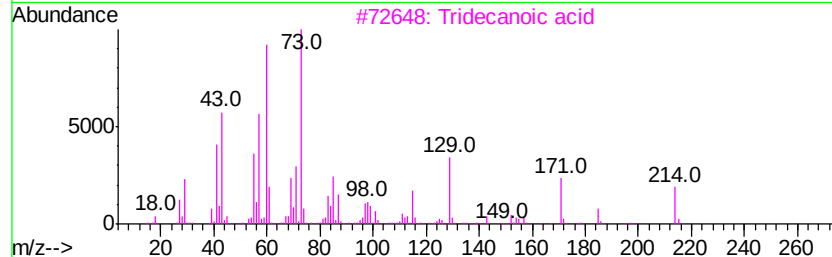
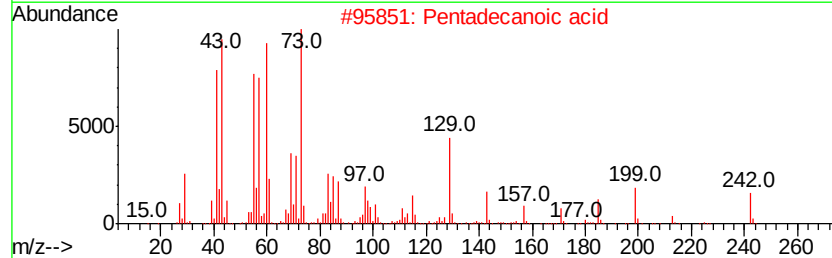
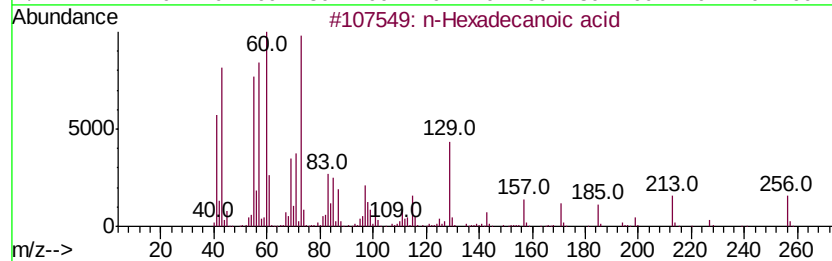
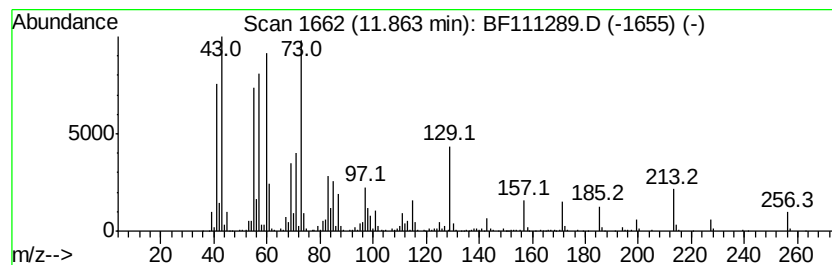
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	23.83 ng	3269440	Phenanthrene-d10	11.32
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 99
2		Pentadecanoic acid	242 C15H30O2	001002-84-2 90
3		Tridecanoic acid	214 C13H26O2	000638-53-9 80
4		Tetradecanoic acid	228 C14H28O2	000544-63-8 80
5		n-Decanoic acid	172 C10H20O2	000334-48-5 64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111289.D
Acq On : 11 Dec 2018 21:14
Operator : JU/SJ
Sample : J6157-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-4-TOTAL

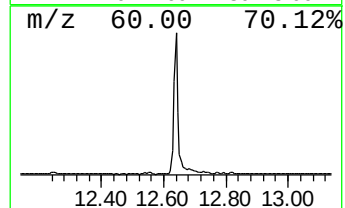
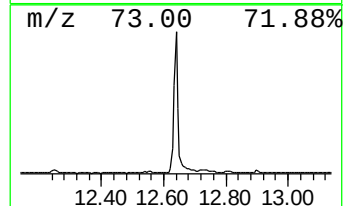
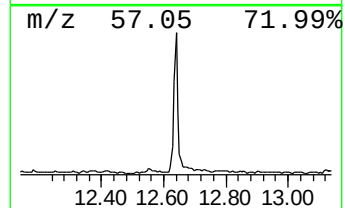
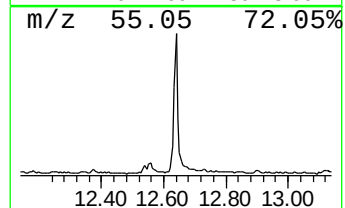
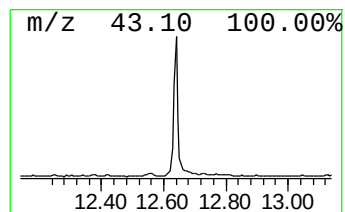
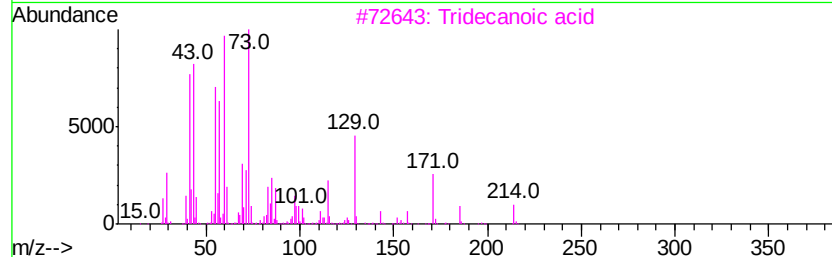
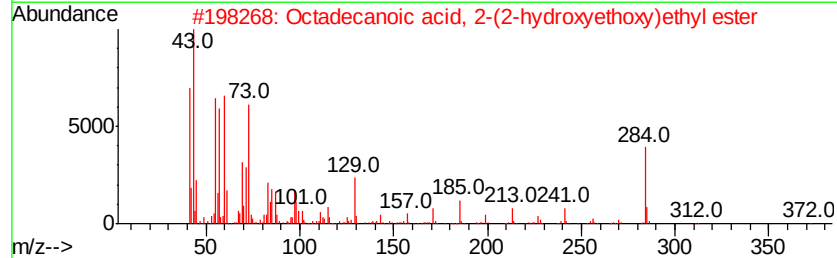
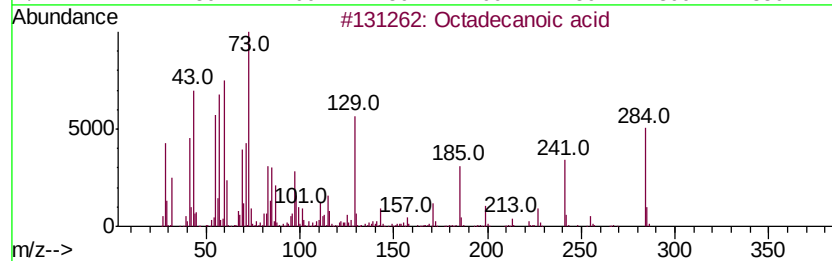
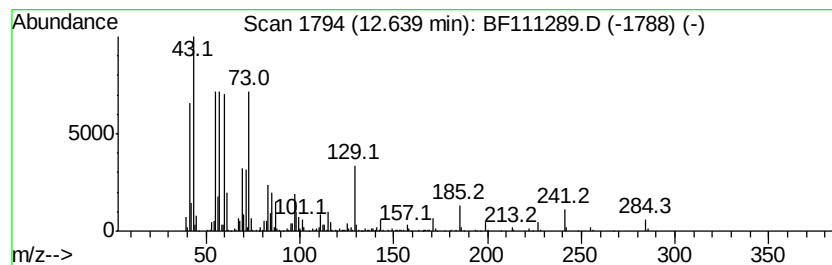
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	16.65 ng	1110280	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	91
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
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 Operator : JU/SJ
 Sample : J6157-07
 Misc :
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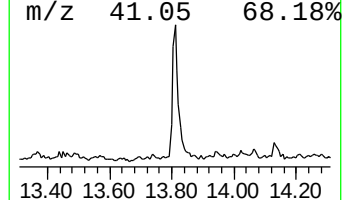
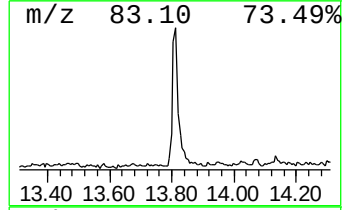
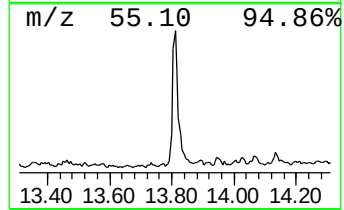
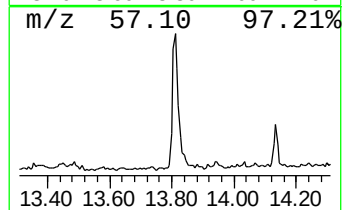
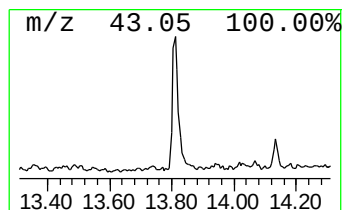
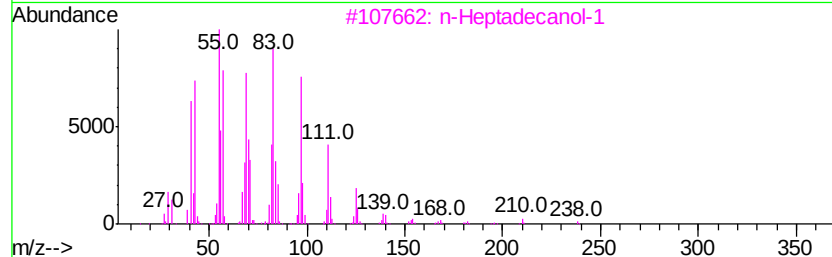
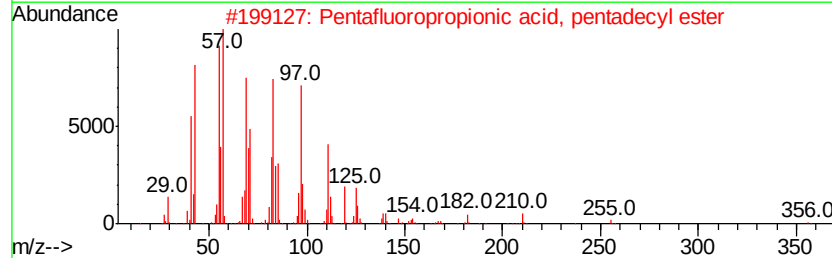
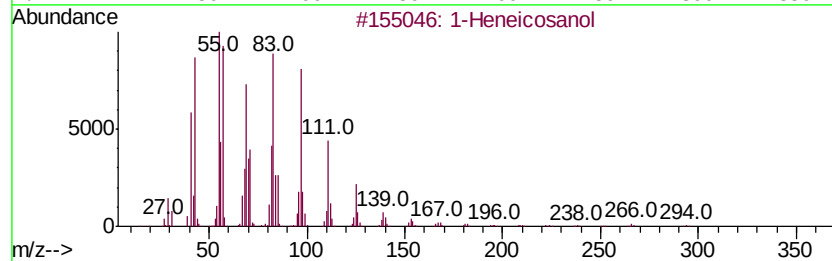
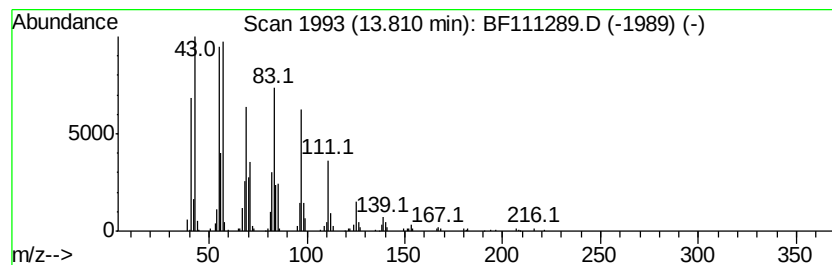
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.81	7.40 ng	493663	Chrysene-d12	13.95		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
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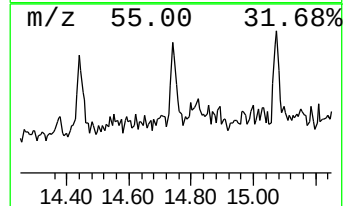
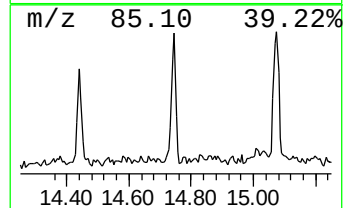
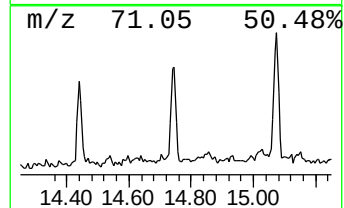
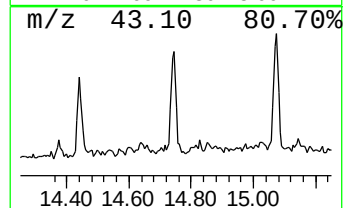
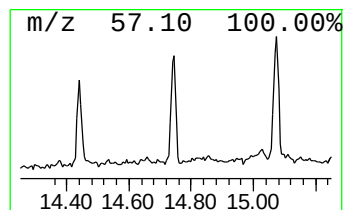
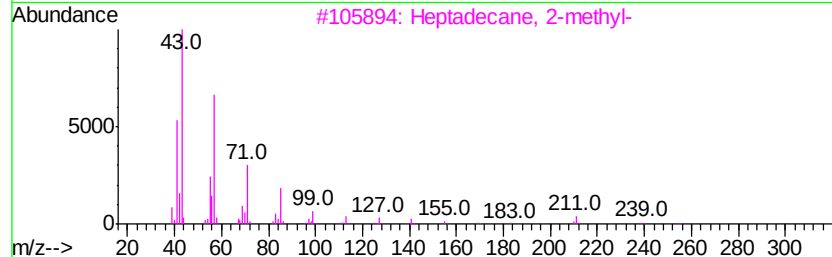
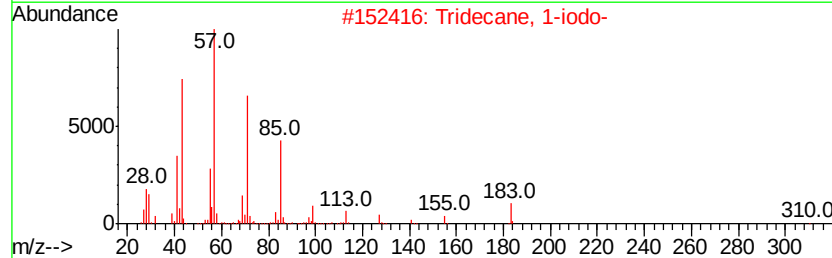
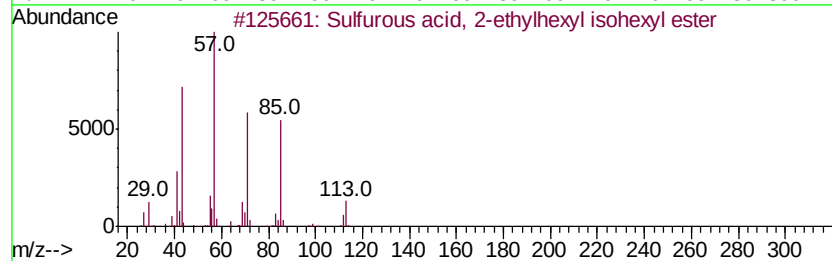
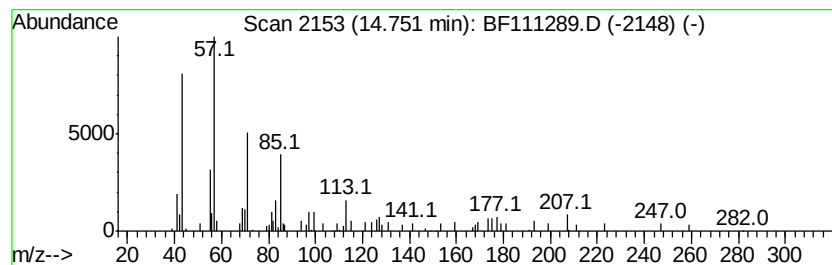
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Sulfurous acid, 2-ethylhexy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.75	2.58 ng	132159	Perylene-d12	15.39		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
3		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	59
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	53
5		Octane, 2-methyl-	128	C9H20	003221-61-2	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111289.D
Acq On : 11 Dec 2018 21:14
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Instrument :
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ClientSampleId :
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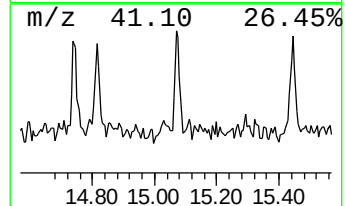
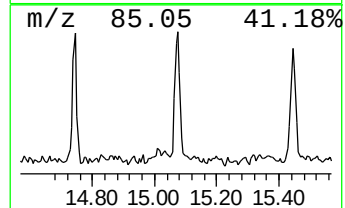
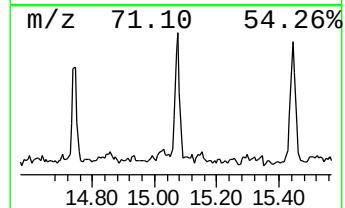
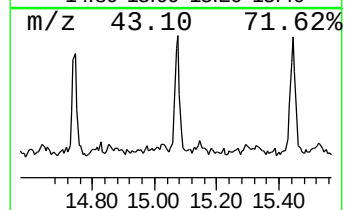
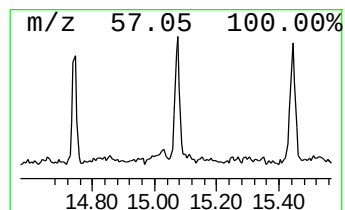
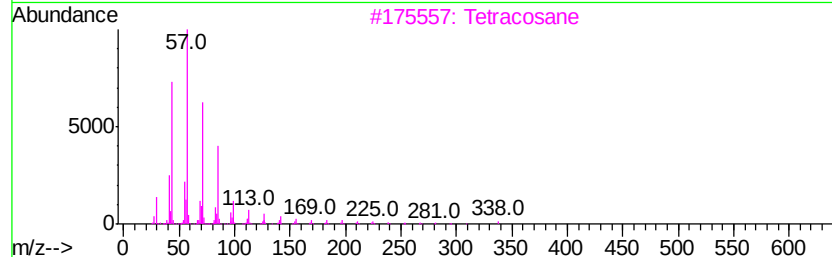
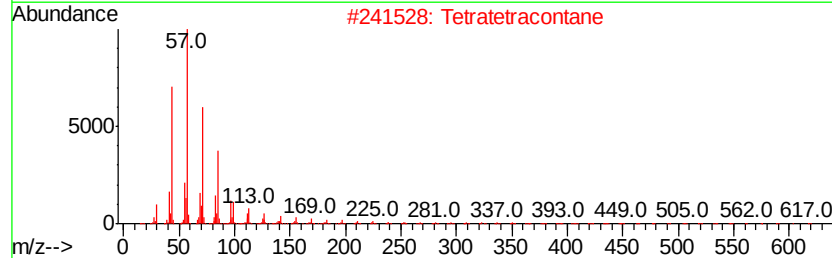
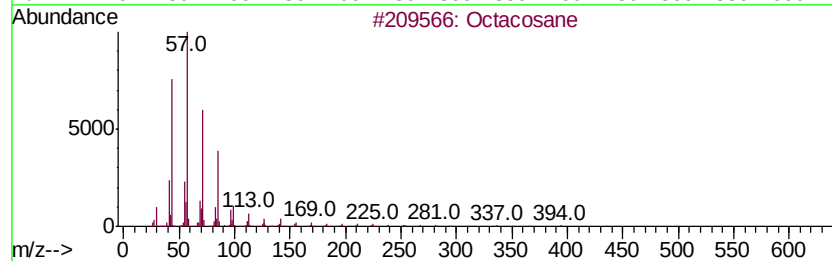
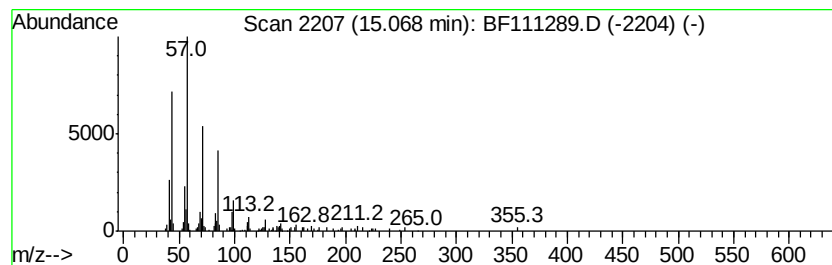
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	2.83 ng	145152	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	91
2		Tetratetracontane	619	C44H90	007098-22-8	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hentriacontane	437	C31H64	000630-04-6	90
5		Hexatriacontane	507	C36H74	000630-06-8	90



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Acq On : 11 Dec 2018 21:14
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ClientSampleId :
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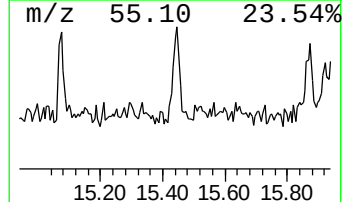
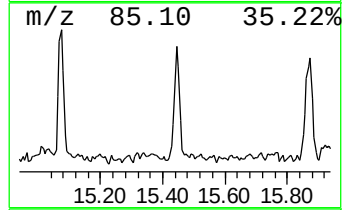
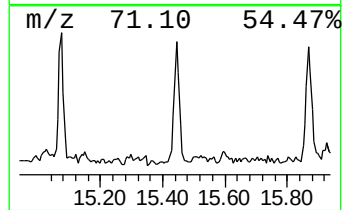
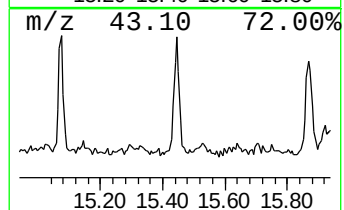
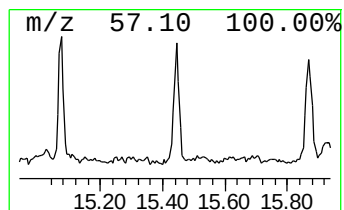
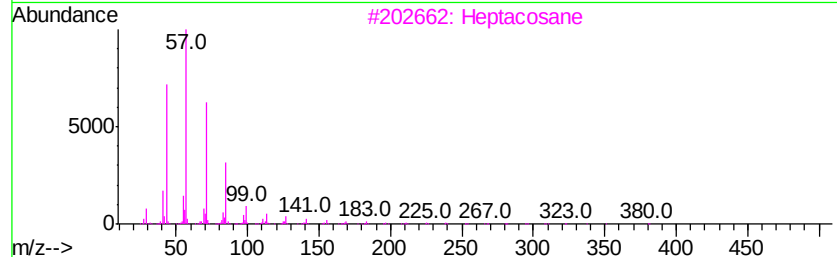
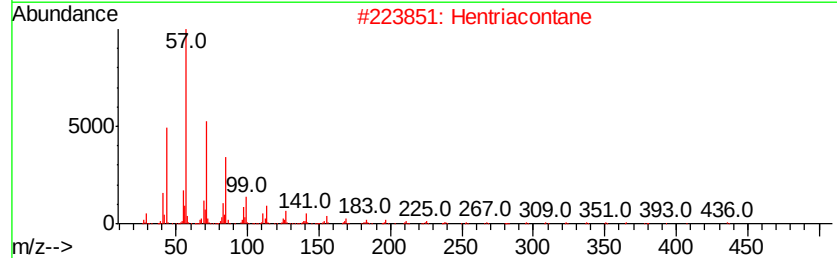
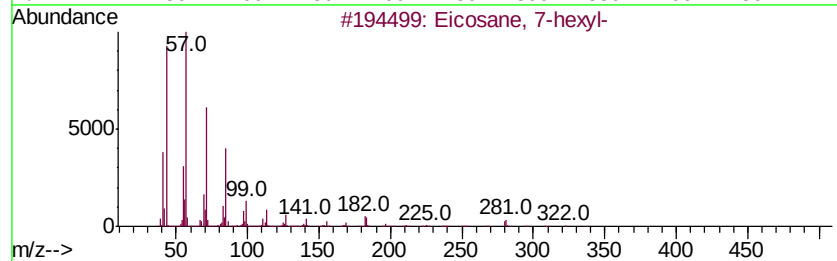
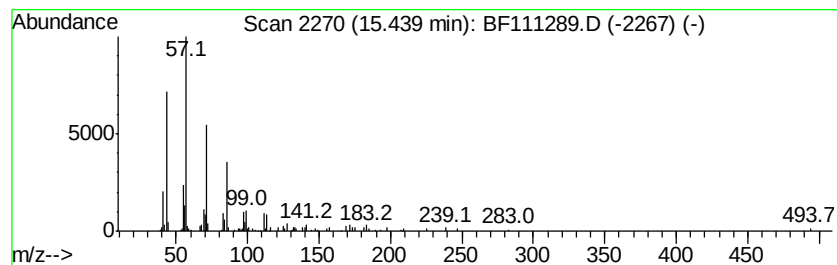
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane, 7-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	3.08 ng	158028	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
2		Hentriacontane	437	C31H64	000630-04-6	87
3		Heptacosane	380	C27H56	000593-49-7	87
4		Eicosane	282	C20H42	000112-95-8	87
5		Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
Data File : BF111289.D
Acq On : 11 Dec 2018 21:14
Operator : JU/SJ
Sample : J6157-07
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMPOSITE-4-TOTAL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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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3-Penten-2-one, 4...	4.36	5.0	ng	445981	1	6.79	1793030	20.0
2-Pentanone, 4-hy...	4.99	10.0	ng	897638	1	6.79	1793030	20.0
unknown5.26	5.26	2.2	ng	198019	1	6.79	1793030	20.0
unknown6.56	6.56	26.6	ng	2389250	1	6.79	1793030	20.0
n-Hexadecanoic acid	11.86	23.8	ng	3269440	4	11.32	2743690	20.0
Octadecanoic acid	12.64	16.6	ng	1110280	5	13.95	1333670	20.0
1-Heneicosanol	13.81	7.4	ng	493663	5	13.95	1333670	20.0
Sulfurous acid, 2...	14.75	2.6	ng	132159	6	15.39	1024890	20.0
Octacosane	15.07	2.8	ng	145152	6	15.39	1024890	20.0
Eicosane, 7-hexyl-	15.44	3.1	ng	158028	6	15.39	1024890	20.0