

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111294.D
 Acq On : 11 Dec 2018 23:44
 Operator : JU/SJ
 Sample : J6157-12
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMPOSITE-6-DISSOLVED

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	2.828	119	126	136	rVB	286627	457100	6.54%	0.804%
2	3.440	223	230	239	rBV	254110	429845	6.15%	0.756%
3	4.040	324	332	336	rBV2	82378	110772	1.58%	0.195%
4	4.369	382	388	392	rBV	4592951	5700826	81.56%	10.022%
5	4.675	436	440	445	rVB	119007	126844	1.81%	0.223%
6	4.987	486	493	501	rVB2	243358	288536	4.13%	0.507%
7	5.404	560	564	572	rBV	2321978	2090214	29.90%	3.675%
8	5.916	648	651	655	rVB	100176	91948	1.32%	0.162%
9	6.422	733	737	748	rBV2	1610739	2454991	35.12%	4.316%
10	6.563	757	761	764	rBV	4709155	3822565	54.69%	6.720%
11	6.792	797	800	804	rBV	2220591	1910348	27.33%	3.358%
12	6.951	823	827	831	rBV	4913648	4339670	62.09%	7.629%
13	7.357	888	896	899	rBV	3655068	3801289	54.38%	6.683%
14	7.504	915	921	926	rBV	177919	200565	2.87%	0.353%
15	8.075	1014	1018	1022	rBV	2511540	2166737	31.00%	3.809%
16	9.157	1197	1202	1205	rBV	7836140	6989880	100.00%	12.288%
17	9.433	1246	1249	1255	rBV	158424	169511	2.43%	0.298%
18	9.545	1264	1268	1271	rBV	1569907	1156084	16.54%	2.032%
19	9.580	1271	1274	1277	rVB	224591	181659	2.60%	0.319%
20	9.704	1292	1295	1298	rBV	81461	80082	1.15%	0.141%
21	9.739	1298	1301	1305	rBV	102785	132002	1.89%	0.232%
22	9.833	1313	1317	1321	rVB	2520931	2328008	33.31%	4.093%
23	10.110	1361	1364	1372	rVB3	107384	123330	1.76%	0.217%
24	10.216	1379	1382	1384	rBV2	74412	76411	1.09%	0.134%
25	10.251	1384	1388	1390	rBV	557816	486840	6.96%	0.856%
26	10.616	1446	1450	1453	rBV	3754832	3334064	47.70%	5.861%
27	11.316	1565	1569	1572	rBV	2695089	2300337	32.91%	4.044%
28	11.851	1656	1660	1670	rBV	1453995	1365830	19.54%	2.401%
29	12.633	1790	1793	1804	rBV	721286	669783	9.58%	1.178%
30	12.904	1834	1839	1842	rBV	6078670	5520522	78.98%	9.705%
31	13.810	1987	1993	1999	rBV2	154820	264294	3.78%	0.465%
32	13.951	2013	2017	2021	rBV	2381021	2123812	30.38%	3.734%
33	14.062	2034	2036	2039	rVB	89267	79307	1.13%	0.139%
34	14.127	2039	2047	2052	rBV3	69419	127742	1.83%	0.225%

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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	14.433	2097	2099	2102	rVB	91304	77455	1.11%	0.136%
36	14.739	2147	2151	2156	rVB2	149643	173352	2.48%	0.305%
37	15.068	2203	2207	2210	rBV	157883	154169	2.21%	0.271%
38	15.386	2256	2261	2266	rBV2	478345	665578	9.52%	1.170%
39	15.439	2266	2270	2275	rVB	131603	197270	2.82%	0.347%
40	15.862	2338	2342	2346	rBV3	76429	111951	1.60%	0.197%

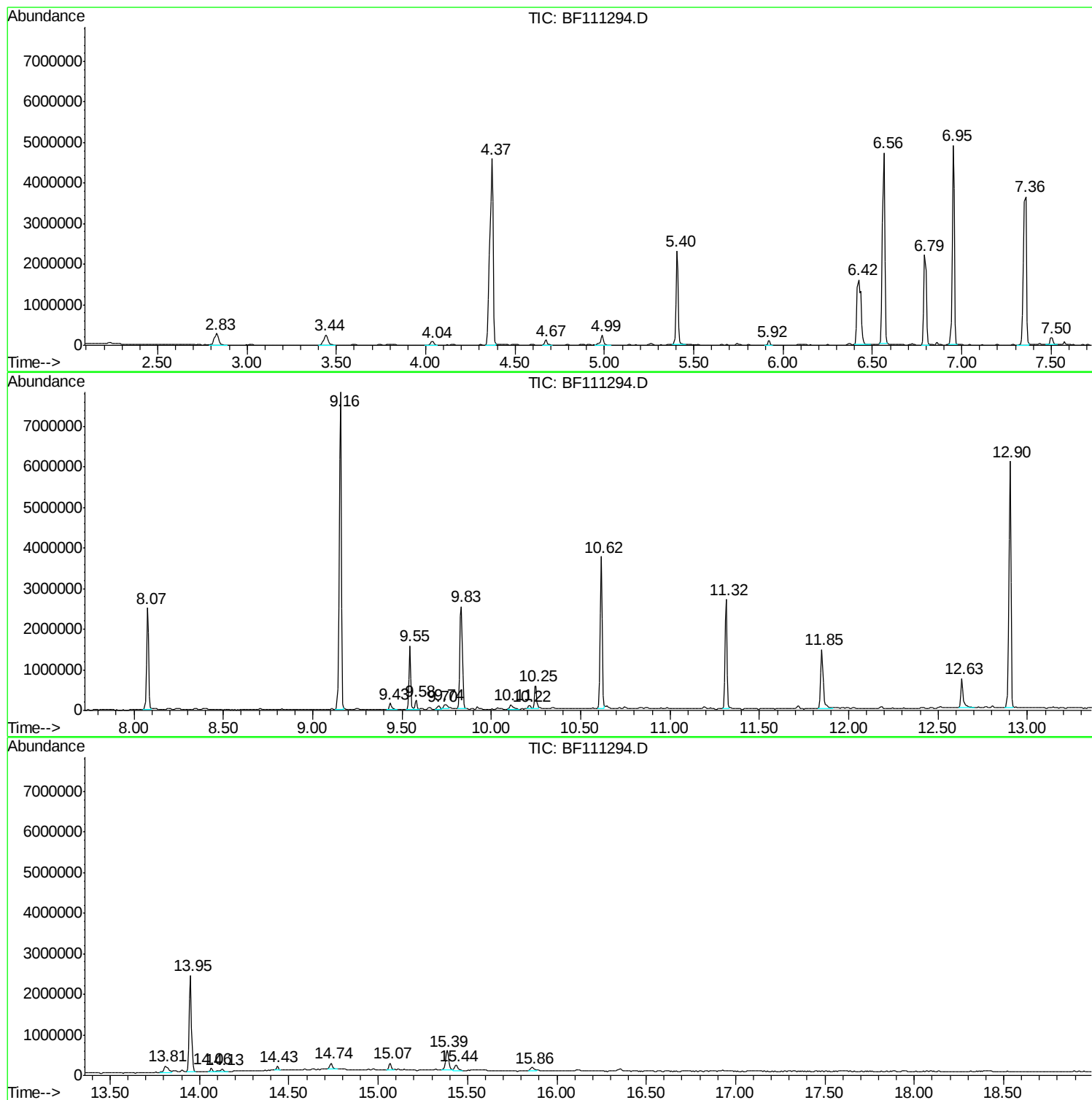
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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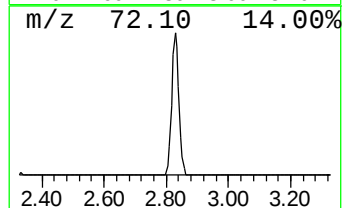
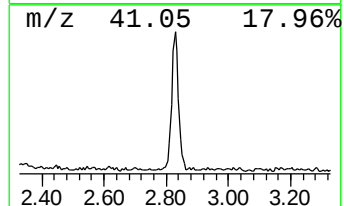
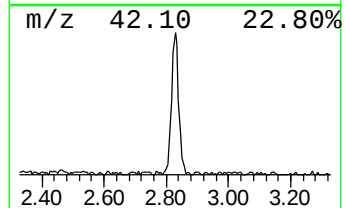
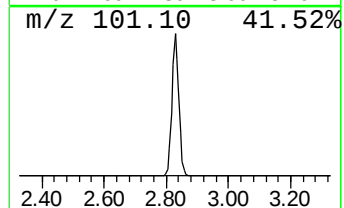
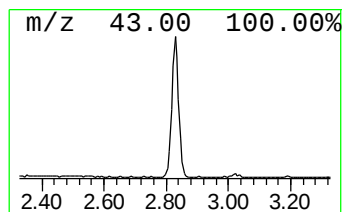
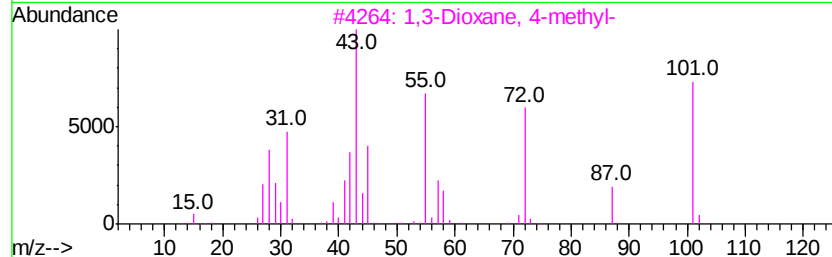
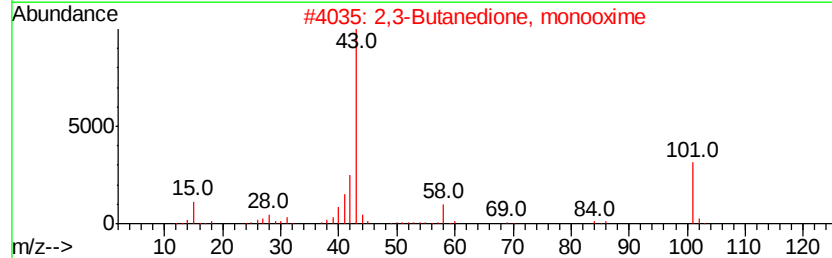
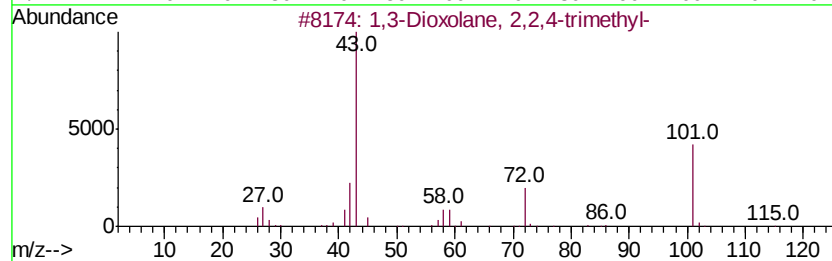
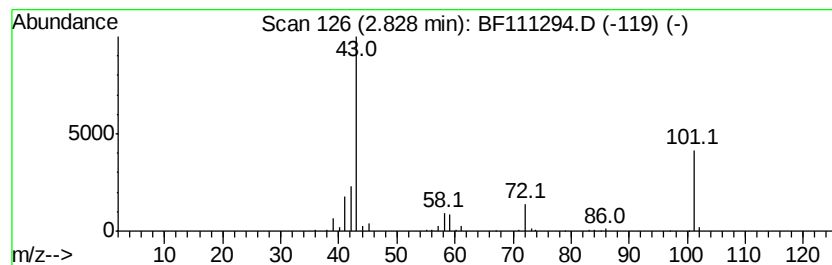
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	4.79 ng	457100	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	64
3		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	36
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9



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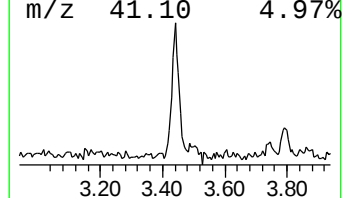
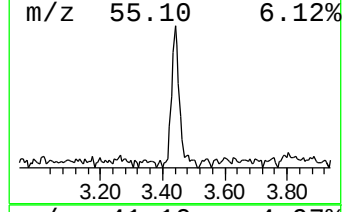
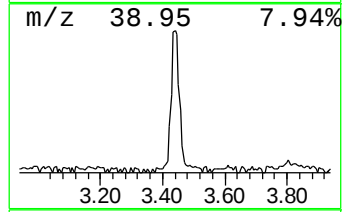
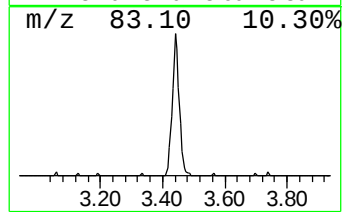
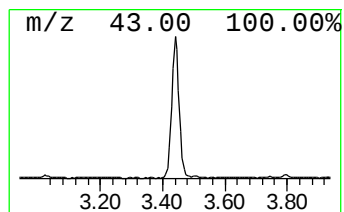
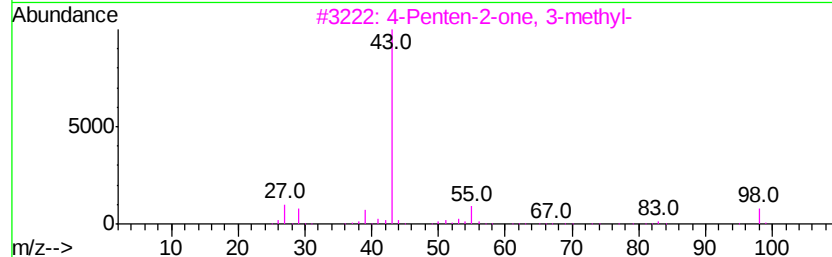
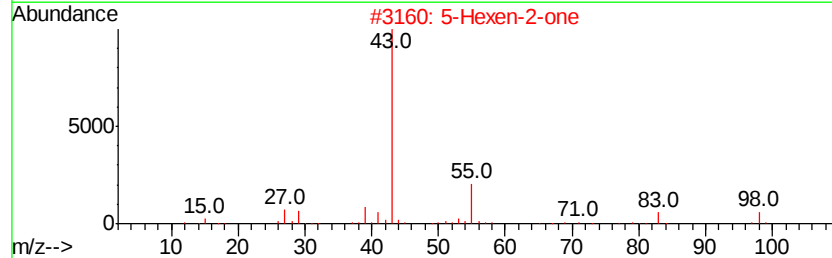
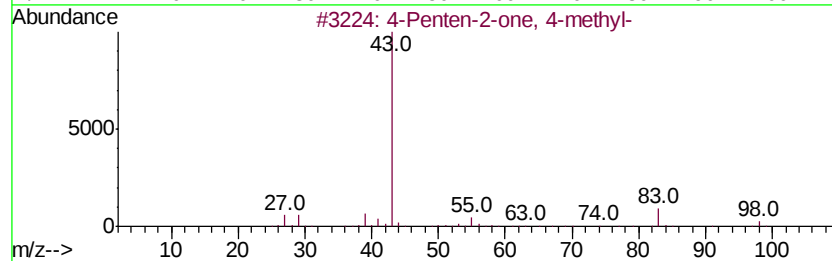
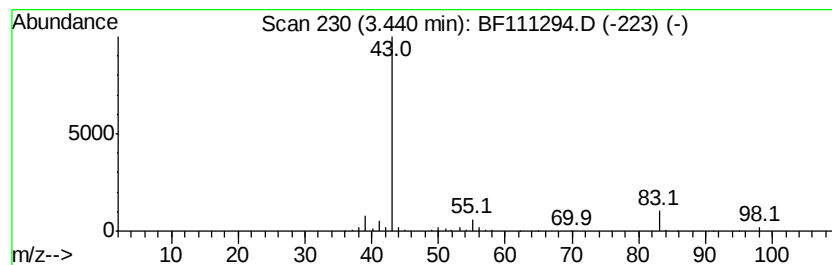
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.44	4.50 ng	429845	1,4-Dichlorobenzene-d4	6.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2			5-Hexen-2-one	98	C6H10O	000109-49-9	38
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	25
4			4-Hexen-2-one	98	C6H10O	025659-22-7	9
5			Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9



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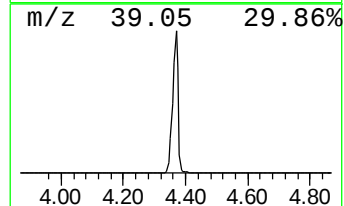
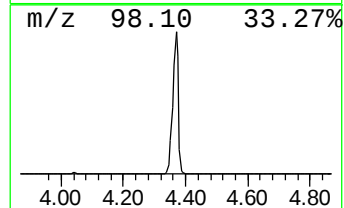
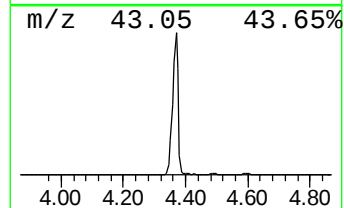
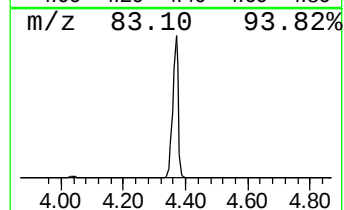
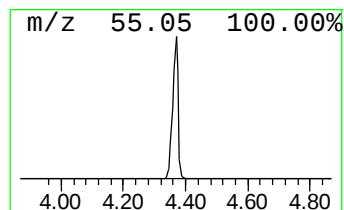
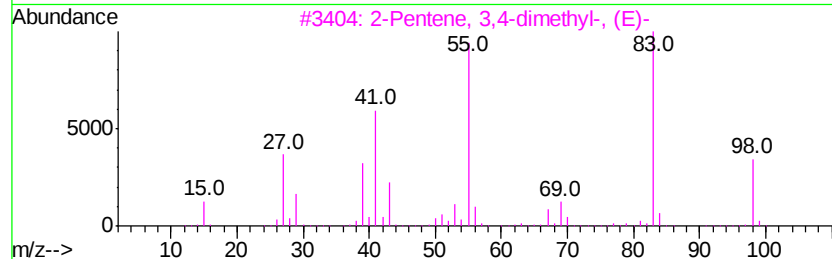
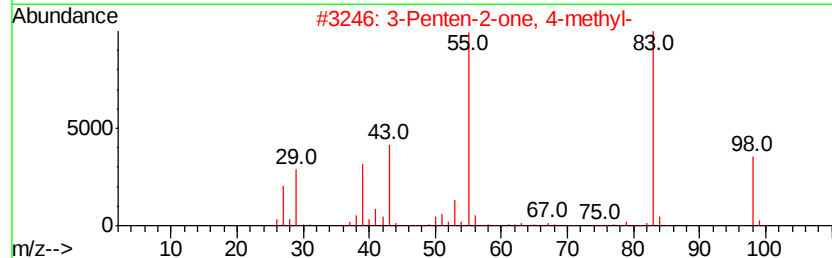
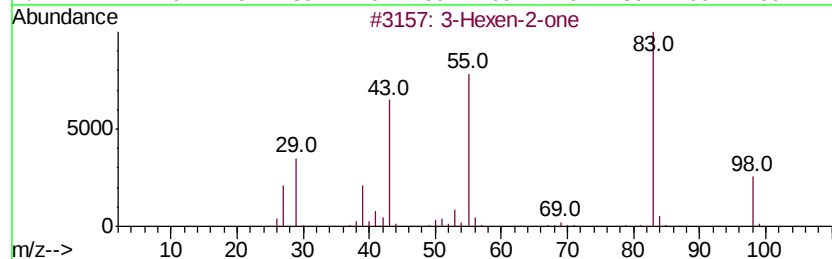
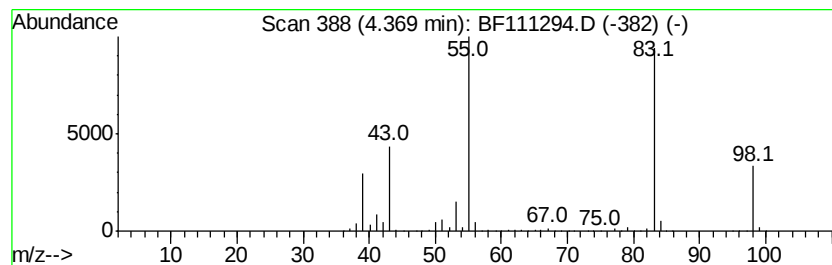
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.37	59.68 ng	5700830	1,4-Dichlorobenzene-d4	6.79

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



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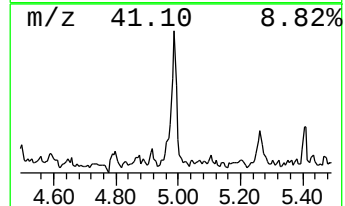
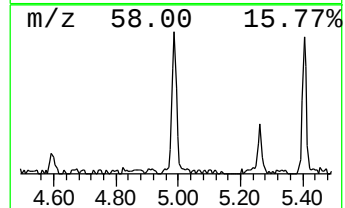
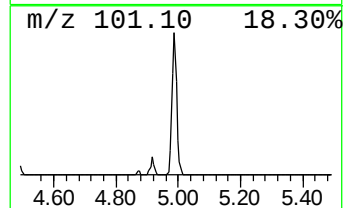
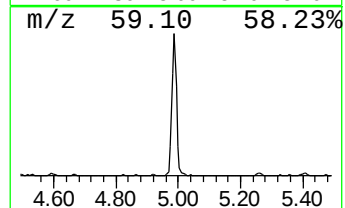
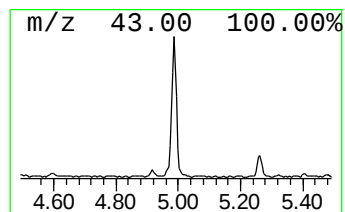
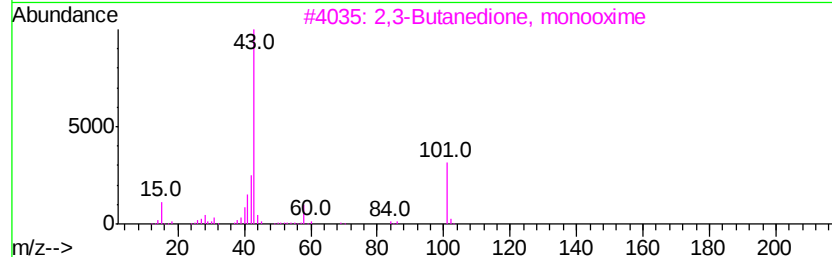
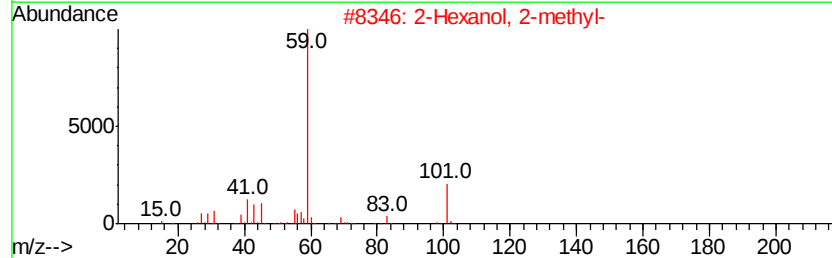
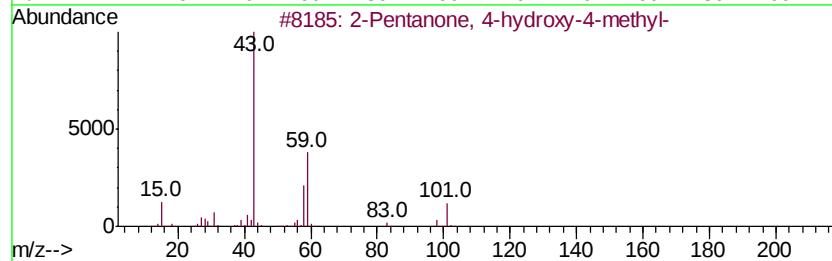
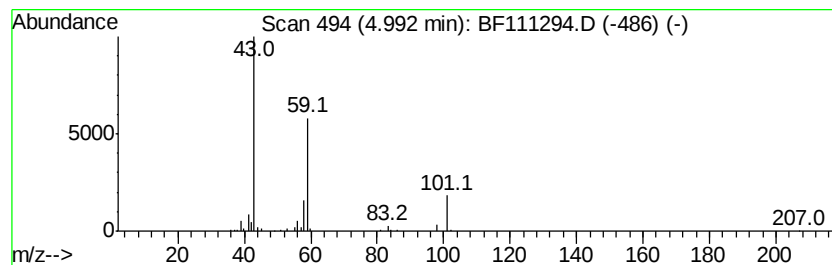
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.02 ng	288536	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	38
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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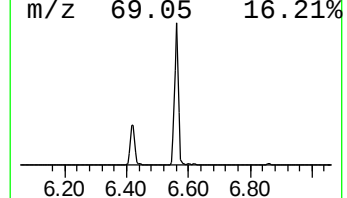
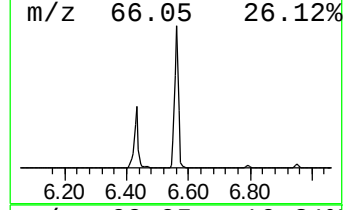
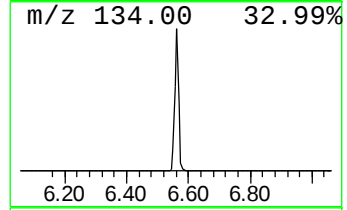
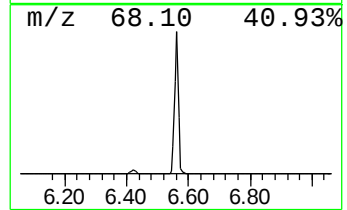
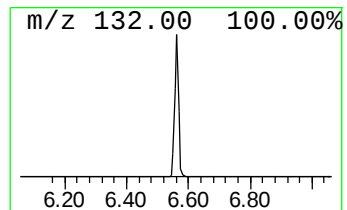
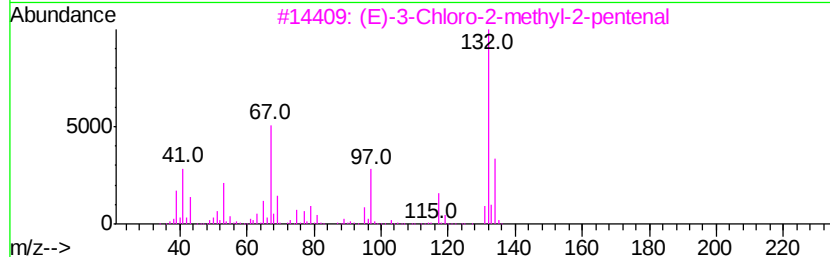
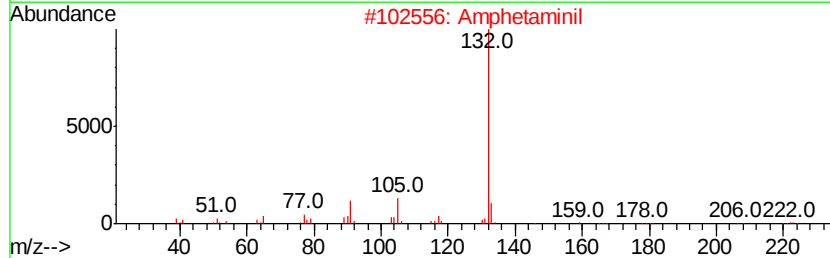
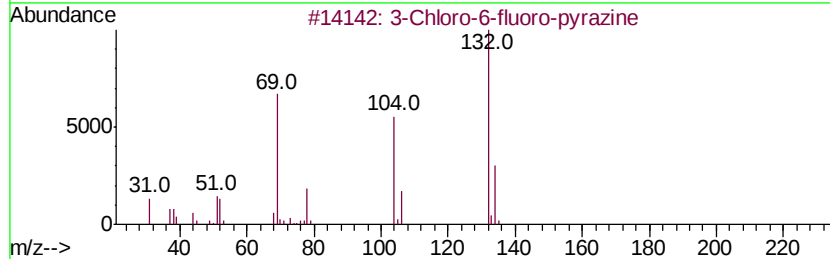
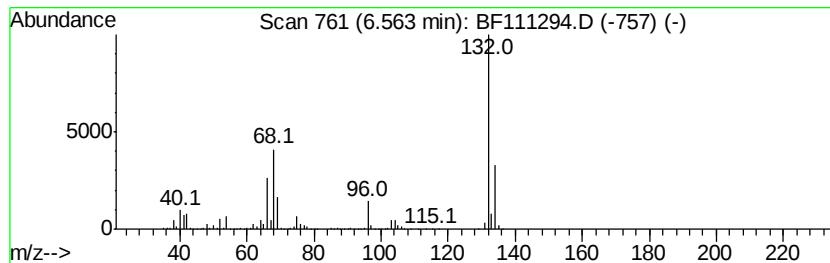
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown6.56 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	40.02 ng	3822570	1,4-Dichlorobenzene-d4	6.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	Amphetaminil	250	C17H18N2	017590-01-1	12	
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12	
5	5-Aminoindole	132	C8H8N2	005192-03-0	9	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111294.D
Acq On : 11 Dec 2018 23:44
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

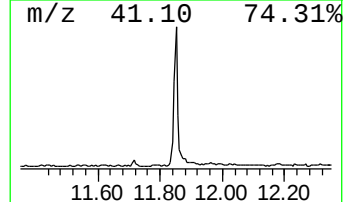
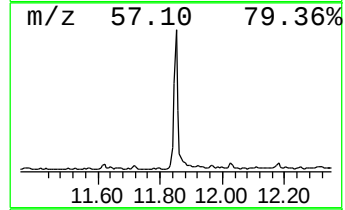
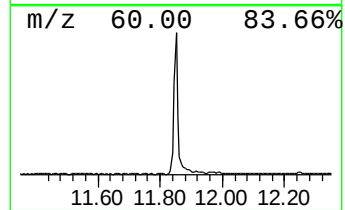
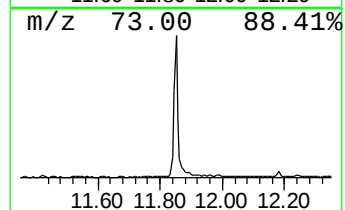
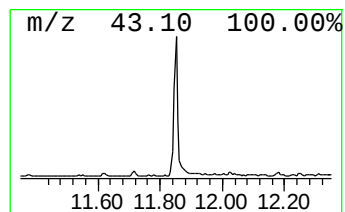
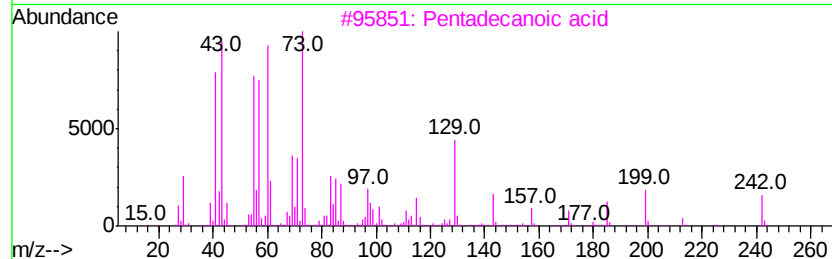
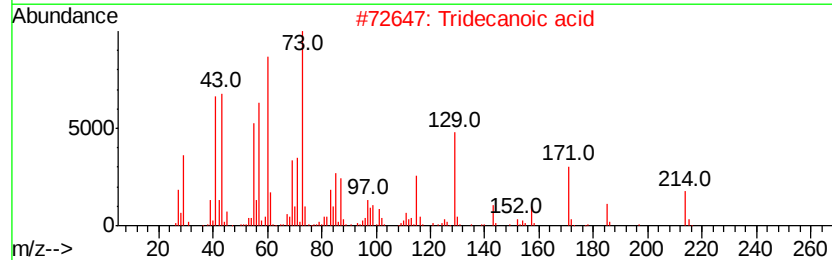
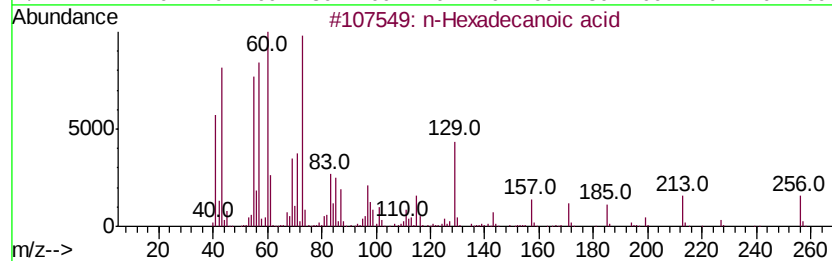
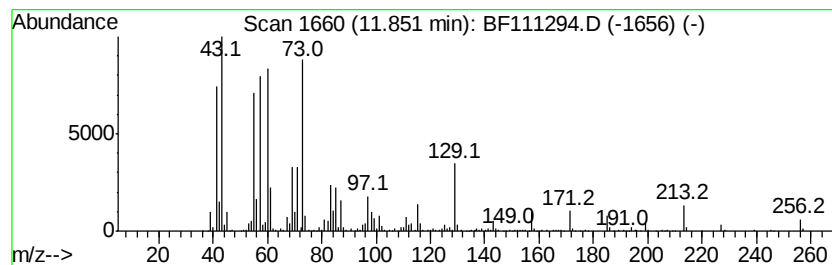
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ClientSampleId :
COMPOSITE-6-DISSOLVED

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 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	11.88 ng	1365830	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111294.D
Acq On : 11 Dec 2018 23:44
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

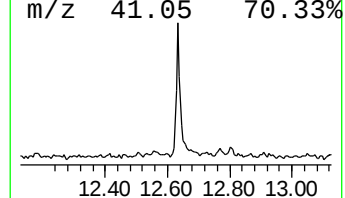
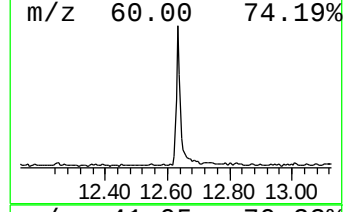
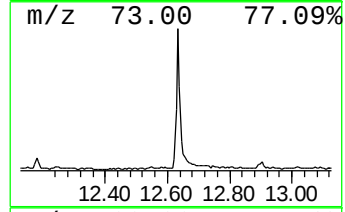
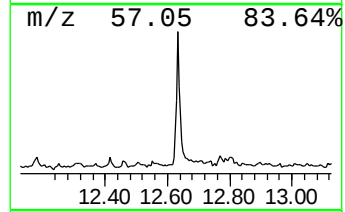
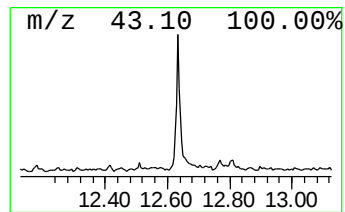
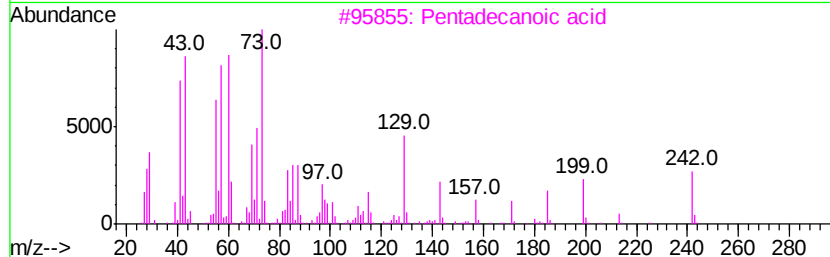
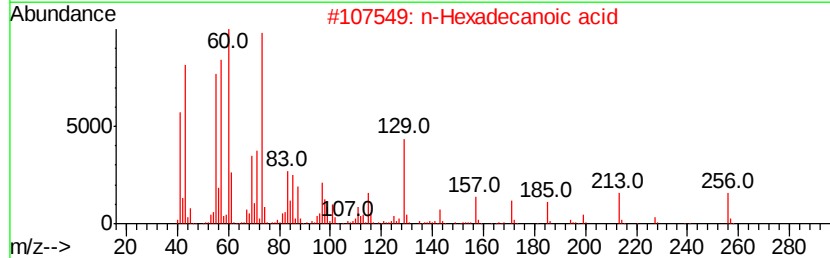
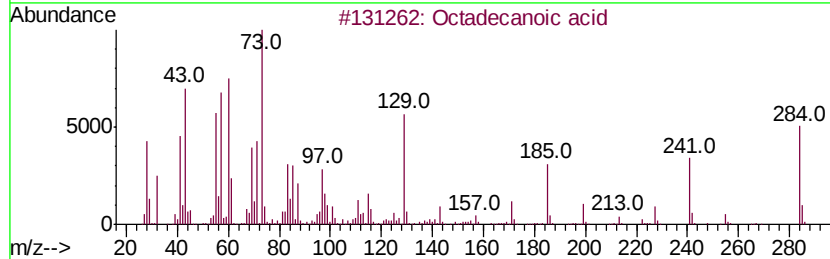
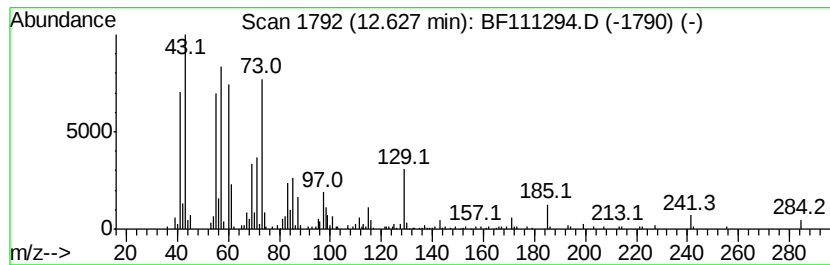
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.63	5.82 ng	669783	Phenanthrene-d10		11.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111294.D
Acq On : 11 Dec 2018 23:44
Operator : JU/SJ
Sample : J6157-12
Misc :
ALS Vial : 13 Sample Multiplier: 1

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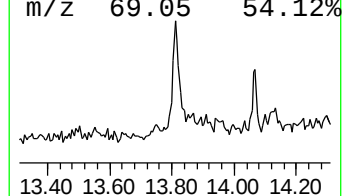
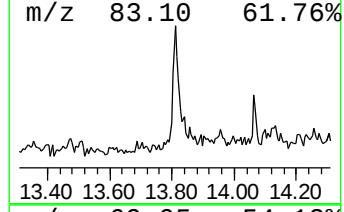
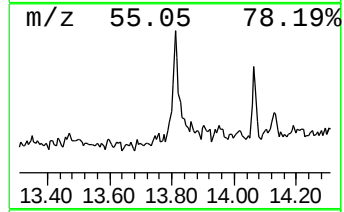
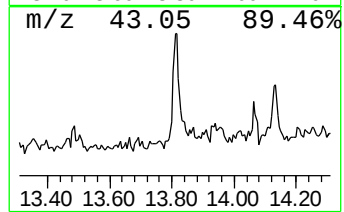
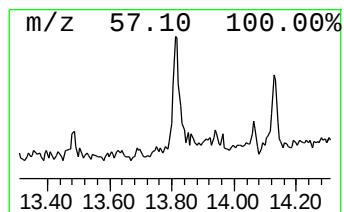
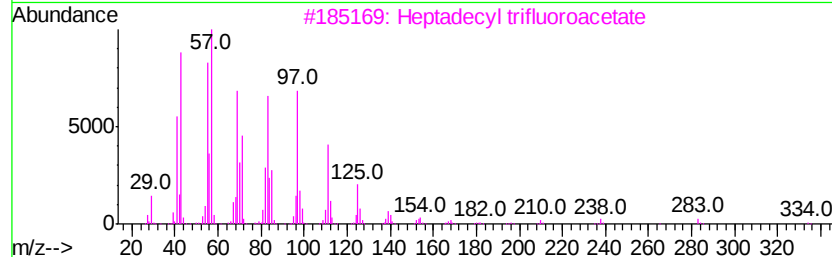
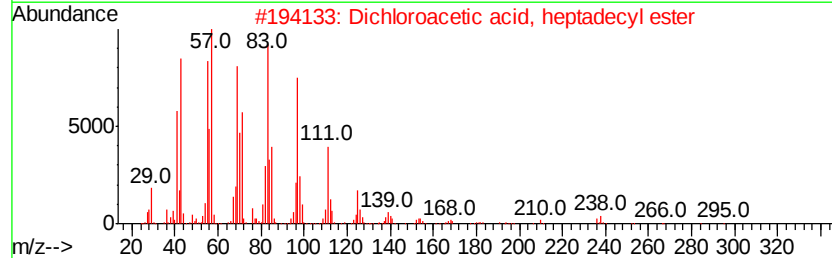
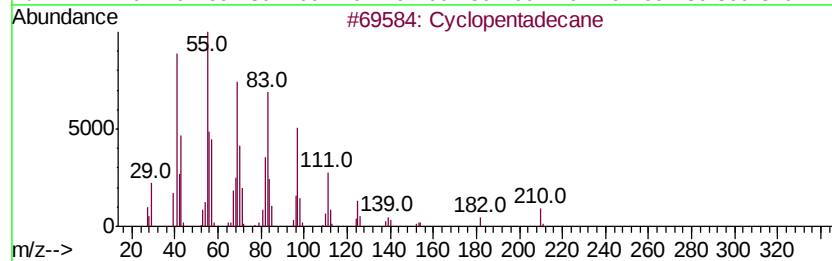
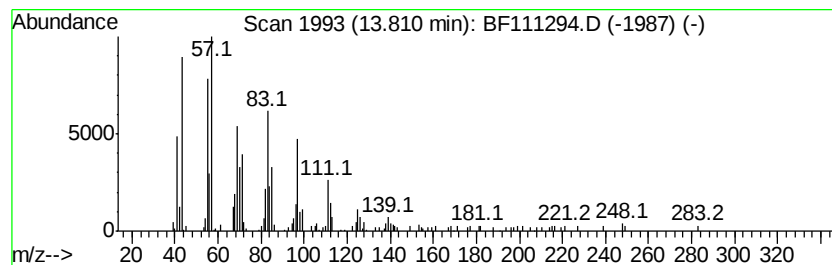
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclopentadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	2.49 ng	264294	Chrysene-d12	13.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	98
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
4		Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	87
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
 Data File : BF111294.D
 Acq On : 11 Dec 2018 23:44
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 ALS Vial : 13 Sample Multiplier: 1

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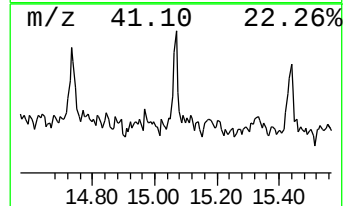
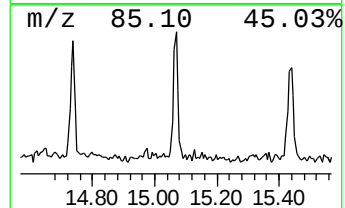
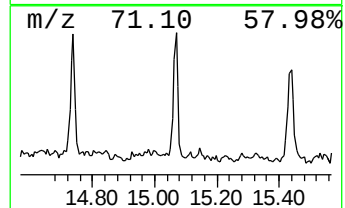
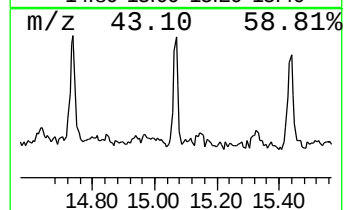
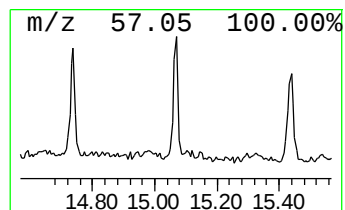
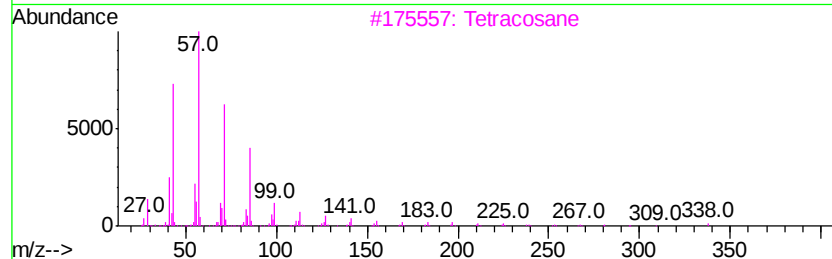
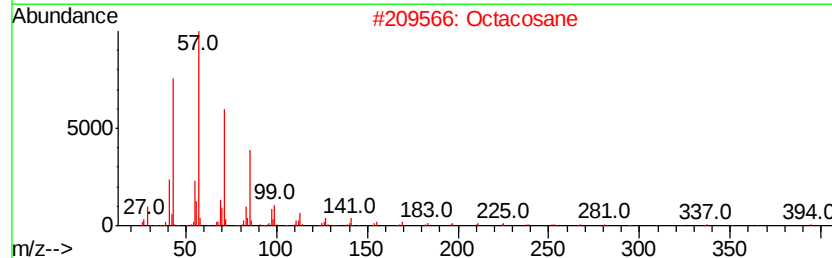
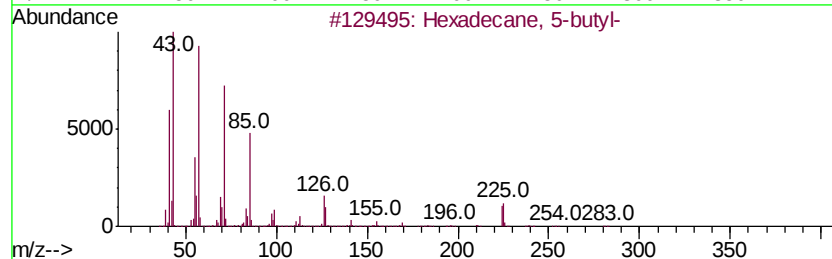
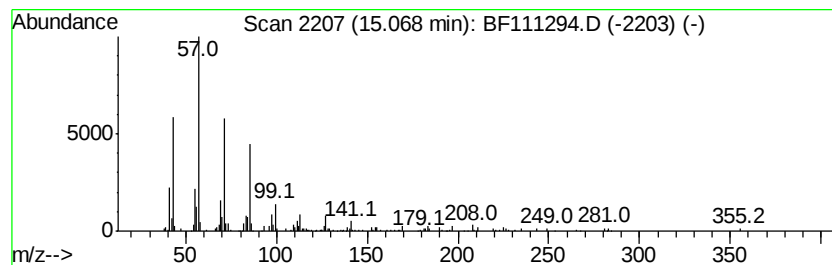
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 Hexadecane, 5-butyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	4.63 ng	154169	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane, 5-butyl-	282	C20H42	006912-07-8	90
2		Octacosane	394	C28H58	000630-02-4	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
5		triacontane	422	C30H62	000638-68-6	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
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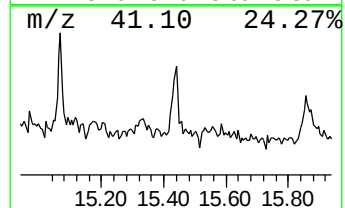
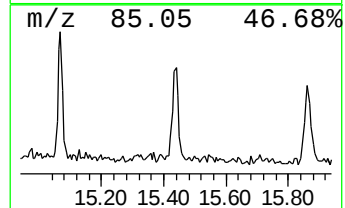
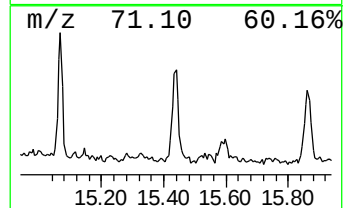
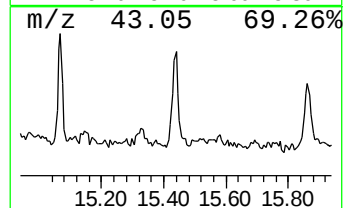
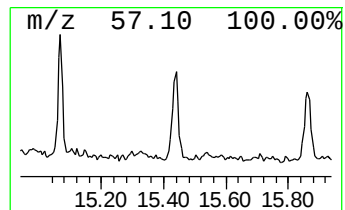
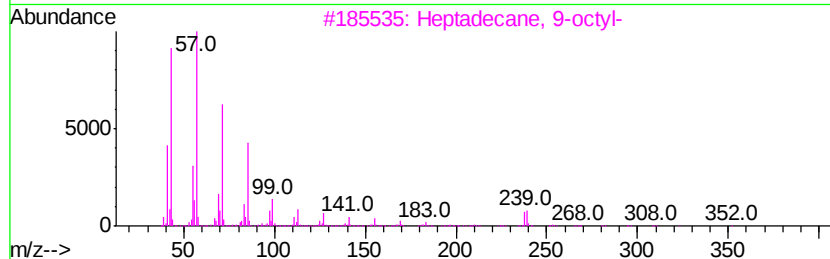
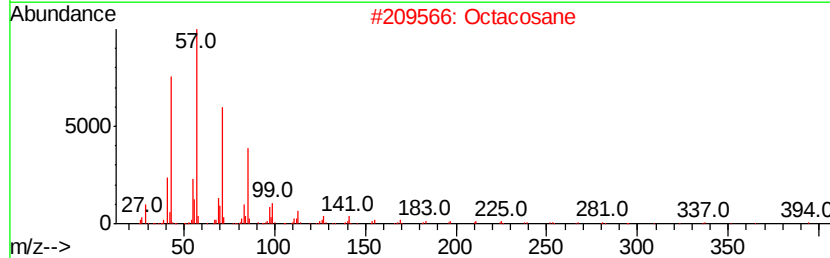
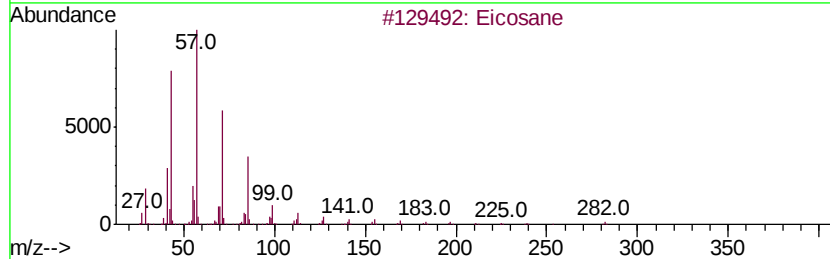
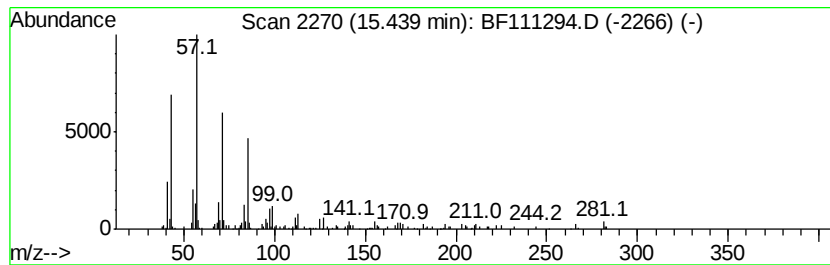
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.44	5.93 ng	197270	Perylene-d12	15.39
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane	282 C20H42	000112-95-8	95
2	Octacosane	394 C28H58	000630-02-4	87
3	Heptadecane, 9-octyl-	352 C25H52	007225-64-1	87
4	Tetracosane	338 C24H50	000646-31-1	80
5	Hentriacontane	437 C31H64	000630-04-6	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111294.D
Acq On : 11 Dec 2018 23:44
Operator : JU/SJ
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ClientSampleId :
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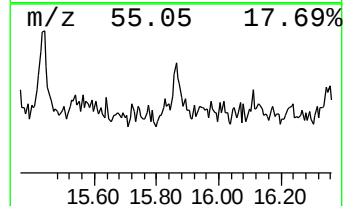
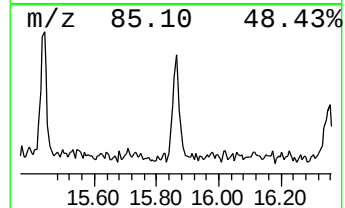
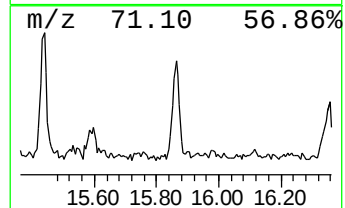
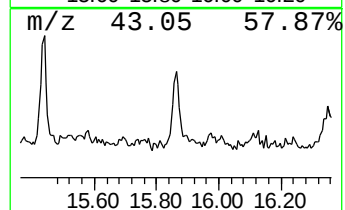
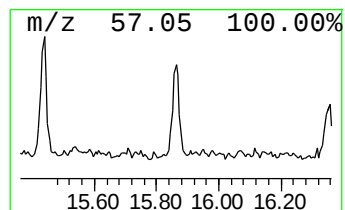
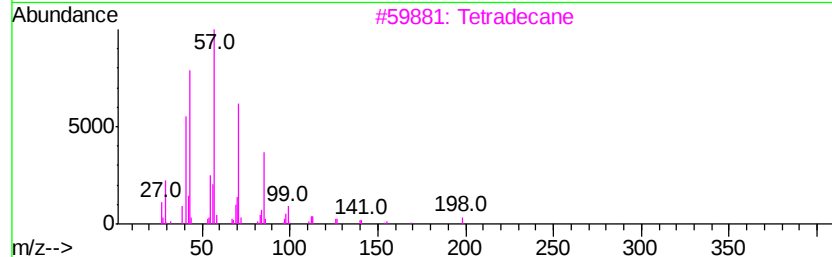
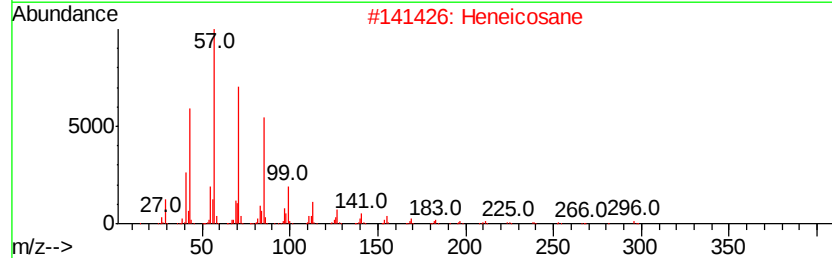
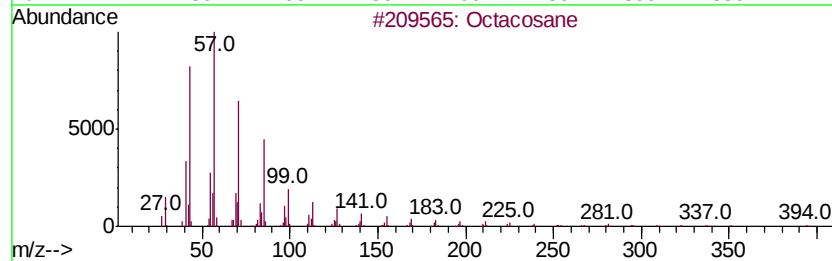
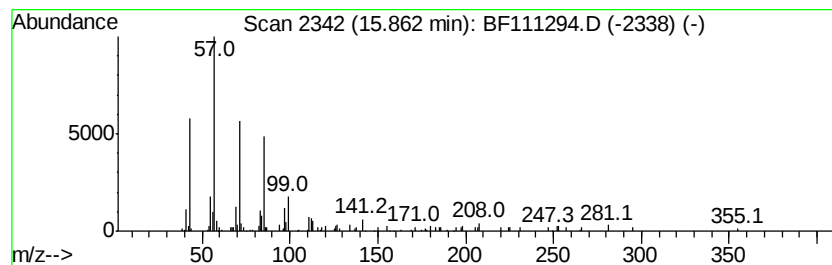
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	3.36 ng	111951	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octacosane	394	C28H58	000630-02-4	86
2		Heneicosane	296	C21H44	000629-94-7	80
3		Tetradecane	198	C14H30	000629-59-4	74
4		Hentriacontane	437	C31H64	000630-04-6	72
5		Pentacosane	352	C25H52	000629-99-2	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
 Data File : BF111294.D
 Acq On : 11 Dec 2018 23:44
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 Sample : J6157-12
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 COMPOSITE-6-DISSOLVED

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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4-Penten-2-one, 4...	3.44	4.5	ng	429845	1	6.79	1910350	20.0
3-Hexen-2-one	4.37	59.7	ng	5700830	1	6.79	1910350	20.0
2-Pentanone, 4-hy...	4.99	3.0	ng	288536	1	6.79	1910350	20.0
unknown6.56	6.56	40.0	ng	3822570	1	6.79	1910350	20.0
n-Hexadecanoic acid	11.85	11.9	ng	1365830	4	11.32	2300340	20.0
Octadecanoic acid	12.63	5.8	ng	669783	4	11.32	2300340	20.0
Cyclopentadecane	13.81	2.5	ng	264294	5	13.95	2123810	20.0
Hexadecane, 5-butyl-	15.07	4.6	ng	154169	6	15.39	665578	20.0
Eicosane	15.44	5.9	ng	197270	6	15.39	665578	20.0
Octacosane	15.86	3.4	ng	111951	6	15.39	665578	20.0