

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
 Data File : BF117515.D
 Acq On : 24 Oct 2019 17:33
 Operator : JU
 Sample : K5499-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 197-16-(0-1)

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-BF101819.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	4.287	371	374	389	rBV	38213	65622	6.56%	0.721%
2	4.939	482	485	499	rBV	22814	31088	3.11%	0.342%
3	5.357	553	556	575	rBV	826240	889651	88.88%	9.776%
4	6.381	727	730	748	rBV	888085	1000960	100.00%	11.000%
5	6.510	748	752	761	rVV	1054701	997746	99.68%	10.964%
6	6.733	787	790	799	rBV	299131	268382	26.81%	2.949%
7	6.886	813	816	827	rBV	723058	619255	61.87%	6.805%
8	7.298	882	886	905	rBV	590962	580385	57.98%	6.378%
9	8.016	1004	1008	1022	rBV	354453	357687	35.73%	3.931%
10	9.086	1186	1190	1203	rBV	949187	787823	78.71%	8.657%
11	9.480	1254	1257	1272	rBB	133240	116447	11.63%	1.280%
12	9.763	1301	1305	1313	rBV	497549	430508	43.01%	4.731%
13	10.557	1436	1440	1452	rBV	516134	484634	48.42%	5.326%
14	11.251	1554	1558	1561	rBV	410038	366803	36.65%	4.031%
15	11.274	1561	1562	1567	rVB	40636	25995	2.60%	0.286%
16	11.780	1645	1648	1656	rBV2	71216	76490	7.64%	0.841%
17	12.463	1761	1764	1769	rBV	50223	51141	5.11%	0.562%
18	12.563	1778	1781	1786	rBV4	9462	13861	1.38%	0.152%
19	12.692	1798	1803	1813	rBV	51446	57454	5.74%	0.631%
20	12.827	1822	1826	1837	rBV	555585	528580	52.81%	5.809%
21	13.027	1853	1860	1862	rBV2	7976	14330	1.43%	0.157%
22	13.257	1896	1899	1901	rBV3	11953	10577	1.06%	0.116%
23	13.727	1976	1979	1990	rBV2	97107	162524	16.24%	1.786%
24	13.862	1999	2002	2004	rBV	29327	27908	2.79%	0.307%
25	13.892	2004	2007	2011	rVV	286843	269690	26.94%	2.964%
26	14.051	2030	2034	2041	rBV4	15747	25769	2.57%	0.283%
27	14.233	2062	2065	2067	rBV2	9907	10144	1.01%	0.111%
28	14.351	2081	2085	2088	rBV4	25274	30764	3.07%	0.338%
29	14.474	2104	2106	2109	rVB	18504	18295	1.83%	0.201%
30	14.651	2133	2136	2141	rVB	36958	36878	3.68%	0.405%
31	14.715	2144	2147	2152	rVV2	34249	37392	3.74%	0.411%
32	14.821	2163	2165	2170	rVB	16981	20178	2.02%	0.222%
33	14.927	2179	2183	2185	rBV	20791	26894	2.69%	0.296%
34	14.962	2186	2189	2193	rVB3	36329	45995	4.60%	0.505%

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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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35	15.098	2209	2212	2213	rBV	13234	12941	1.29%	0.142%
36	15.209	2228	2231	2237	rBV3	16681	23007	2.30%	0.253%
37	15.274	2239	2242	2245	rVV	22884	26596	2.66%	0.292%
38	15.327	2246	2251	2263	rVB	251700	351466	35.11%	3.862%
39	15.509	2280	2282	2285	rBV4	8622	10350	1.03%	0.114%
40	15.727	2314	2319	2325	rBV	36847	54473	5.44%	0.599%
41	15.803	2327	2332	2342	rVV	18080	55457	5.54%	0.609%
42	15.892	2344	2347	2351	rVB	17613	23749	2.37%	0.261%
43	16.192	2394	2398	2402	rBV3	25057	40135	4.01%	0.441%
44	16.733	2487	2490	2491	rBV3	13082	13936	1.39%	0.153%

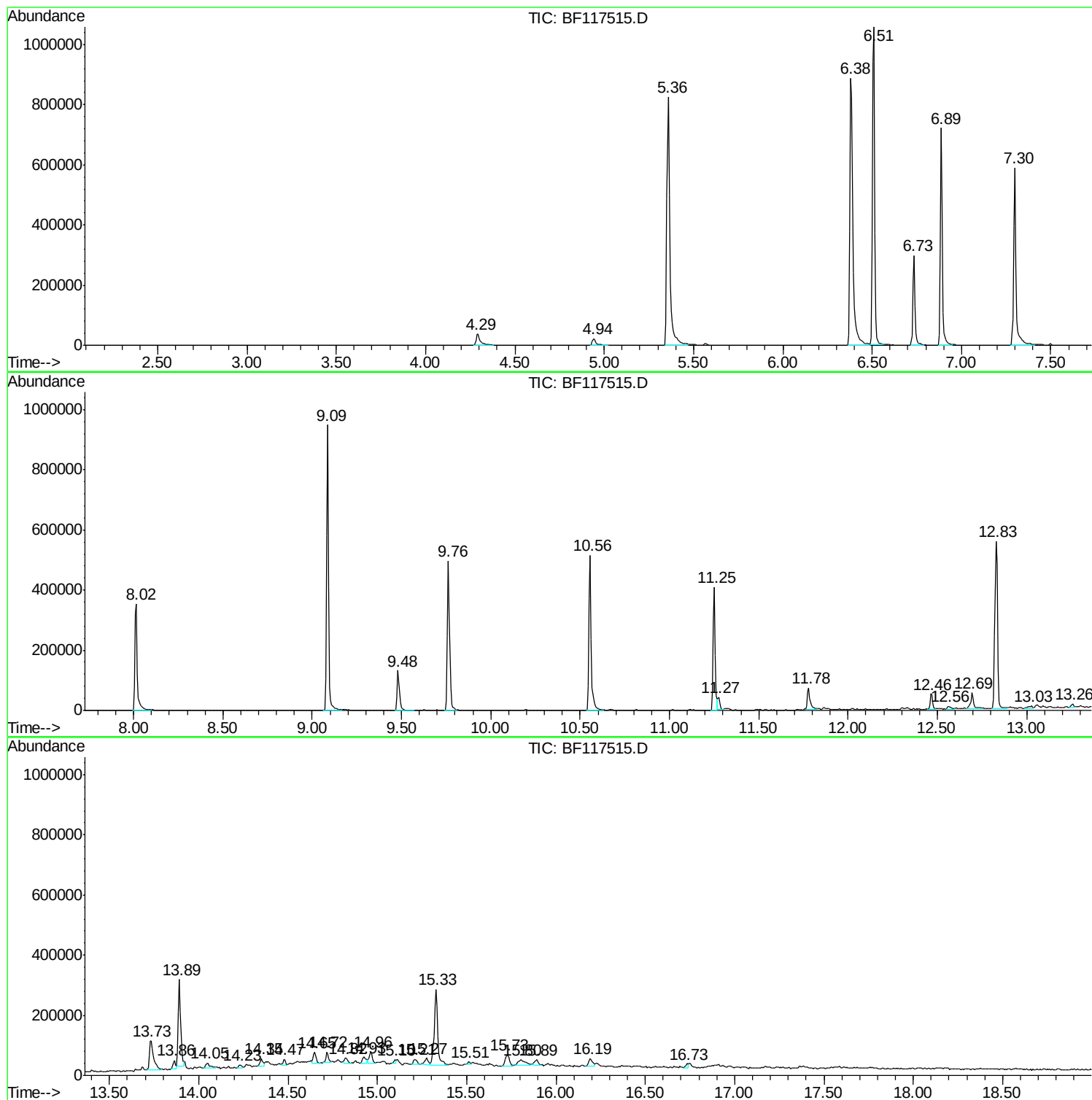
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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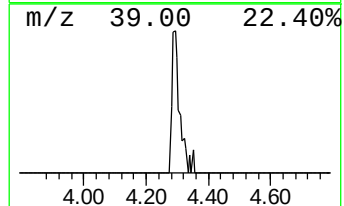
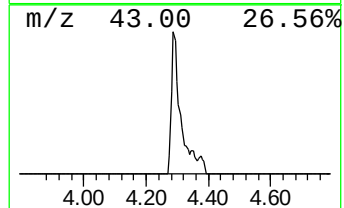
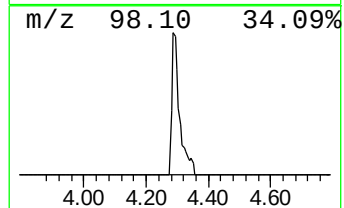
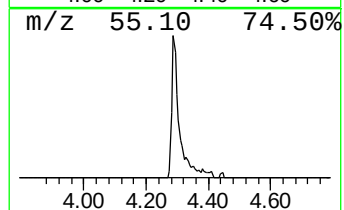
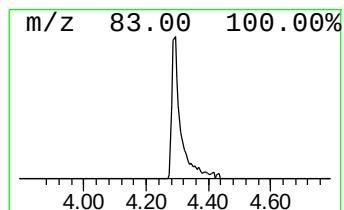
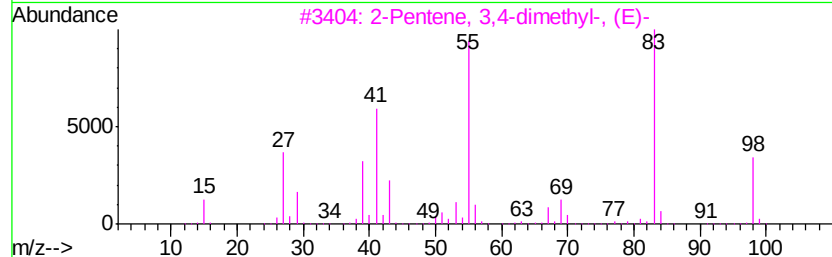
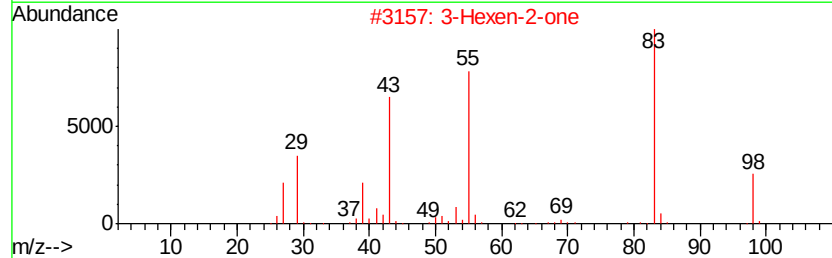
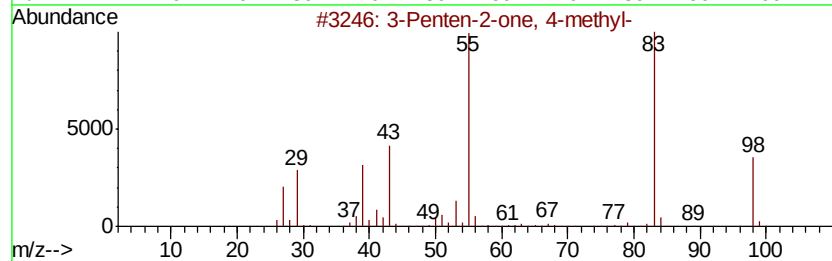
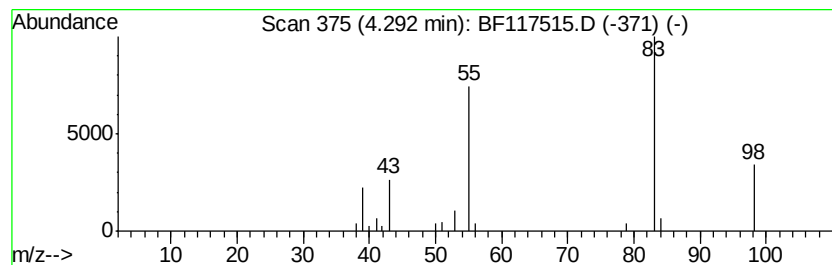
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	4.89 ng	65622	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80



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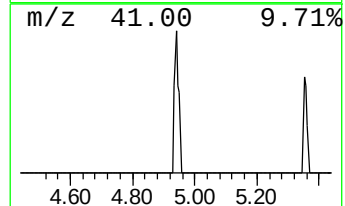
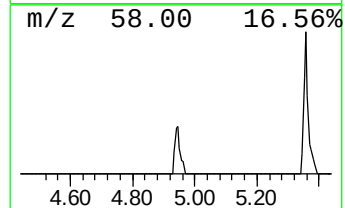
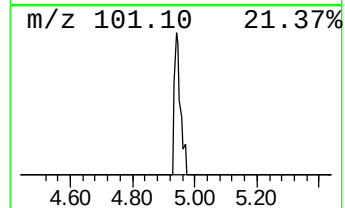
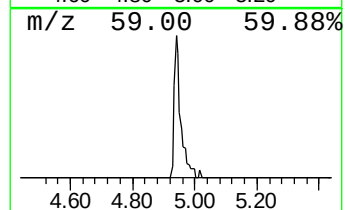
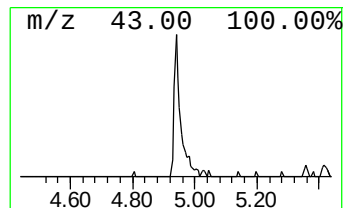
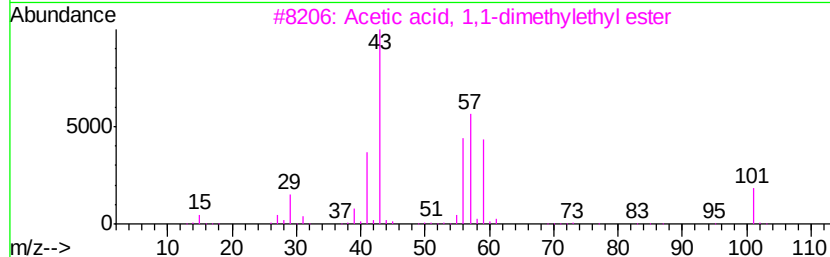
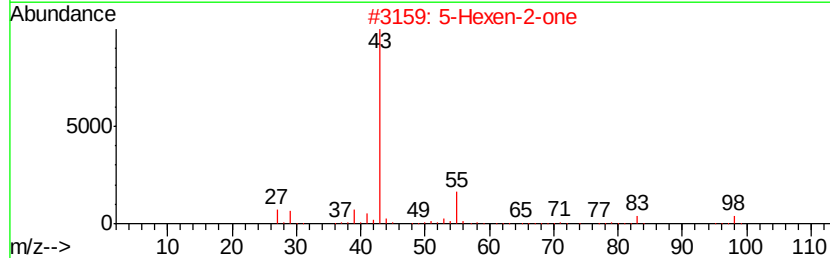
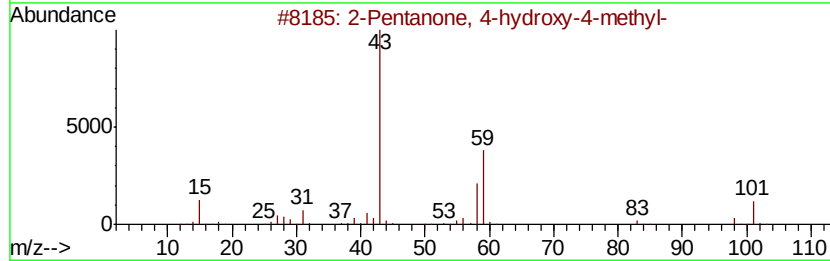
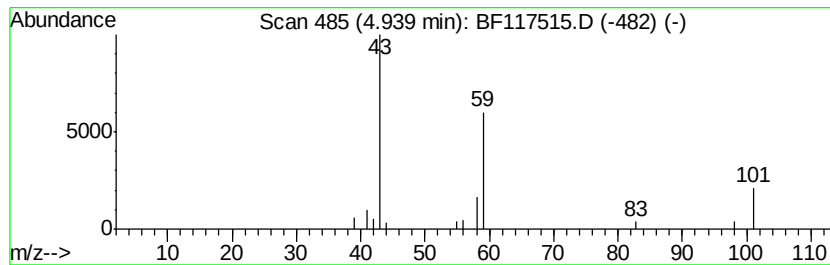
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.94 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	2.32 ng	31088	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
5	2-Nonanone	142	C9H18O	000821-55-6	9		



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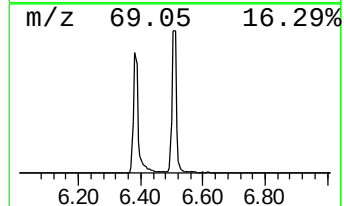
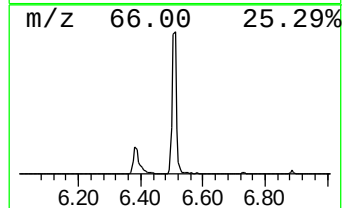
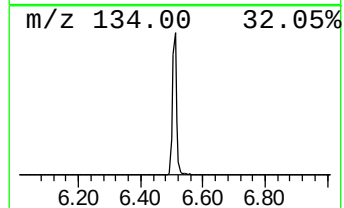
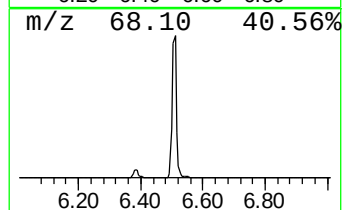
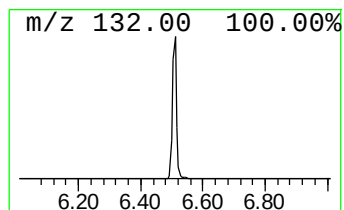
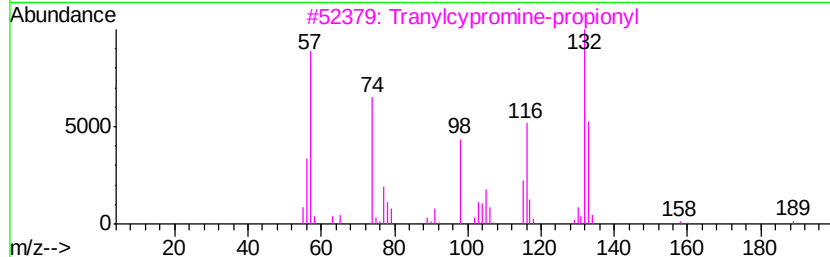
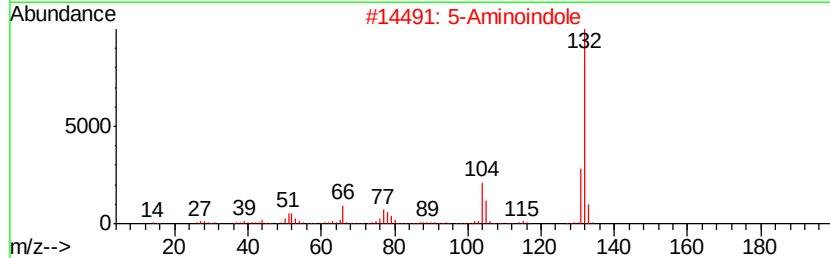
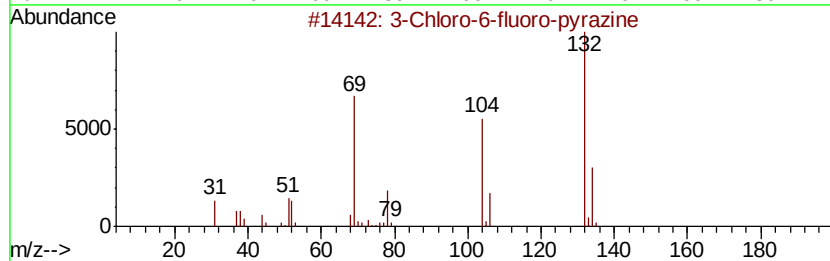
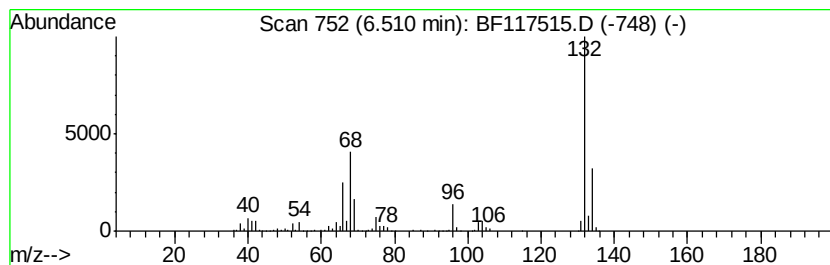
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	74.35 ng	997746	1,4-Dichlorobenzene-d4	6.73

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	22
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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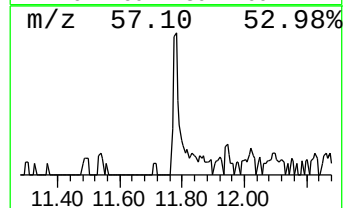
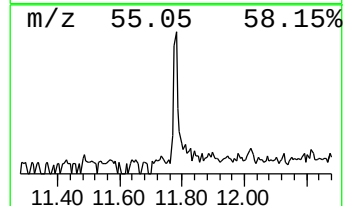
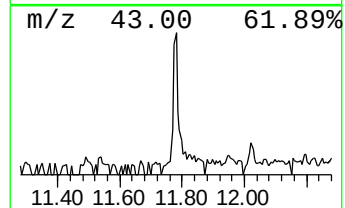
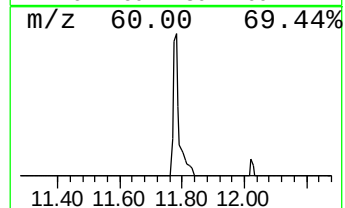
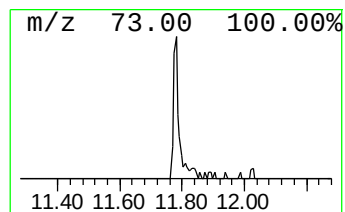
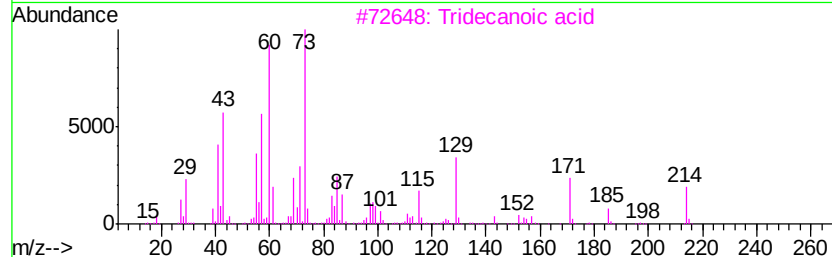
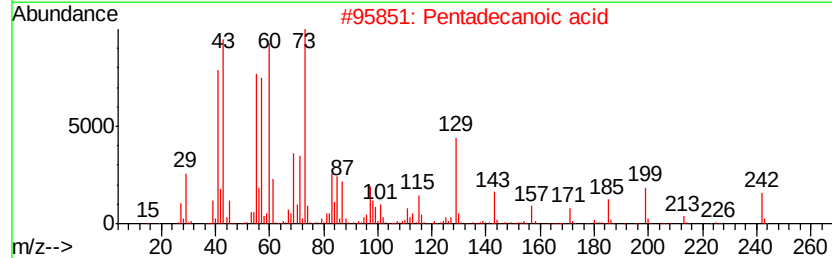
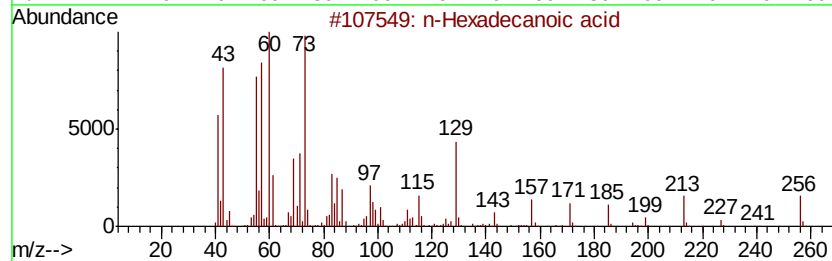
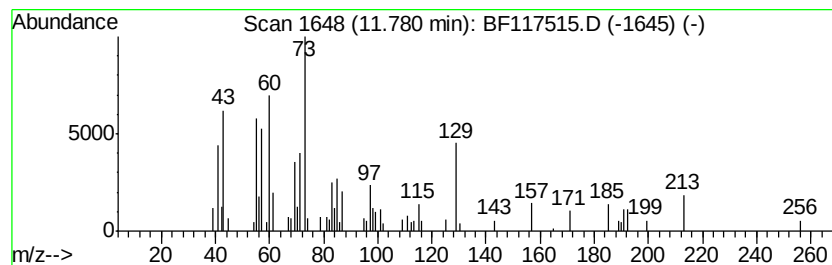
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	4.17 ng	76490	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	.beta.-D-Mannofuranoside, 1-O-(1...	332	C17H32O6	1000155-29-9	27
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	25



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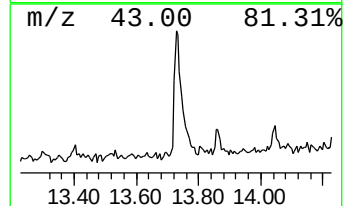
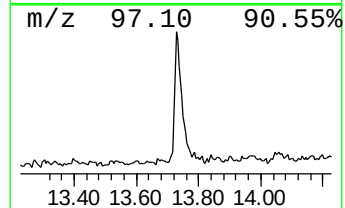
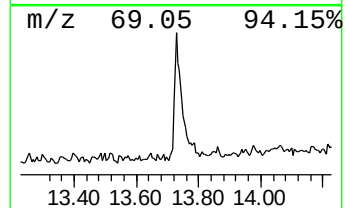
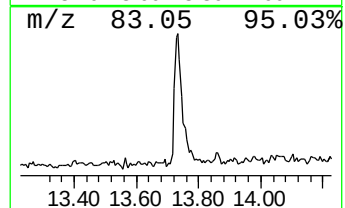
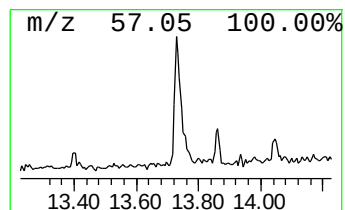
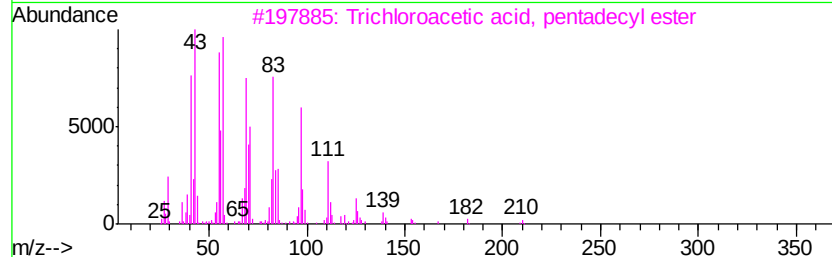
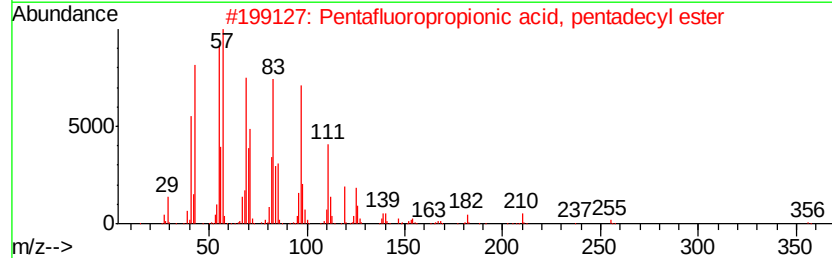
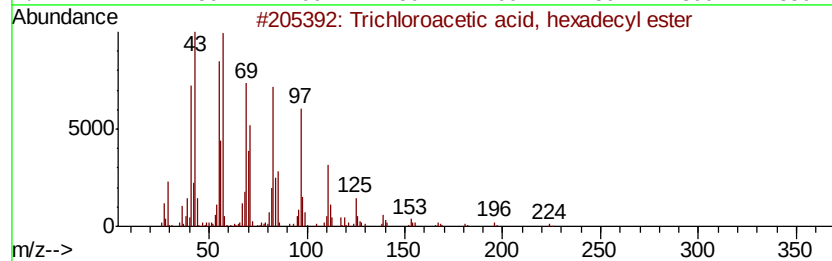
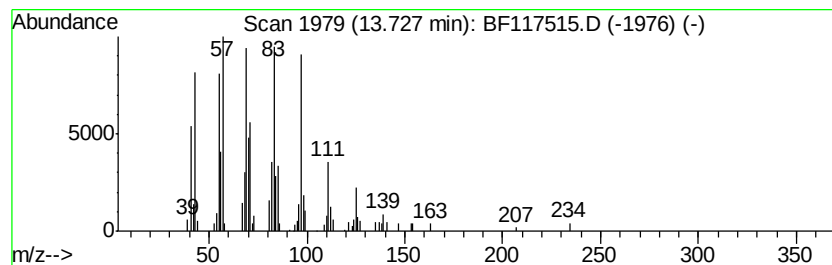
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	12.05 ng	162524	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117515.D
Acq On : 24 Oct 2019 17:33
Operator : JU
Sample : K5499-07
Misc :
ALS Vial : 9 Sample Multiplier: 1

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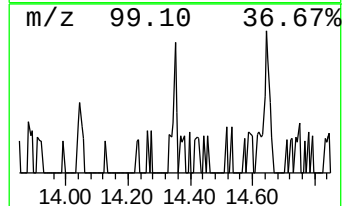
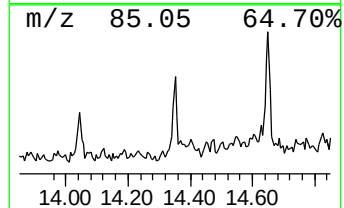
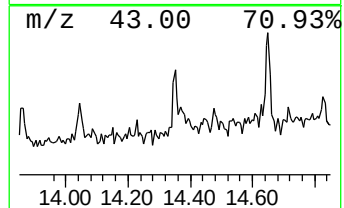
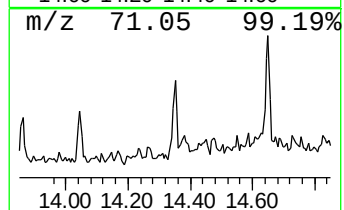
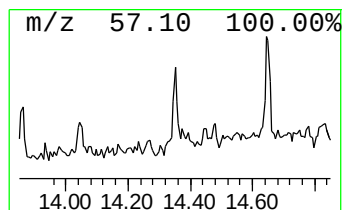
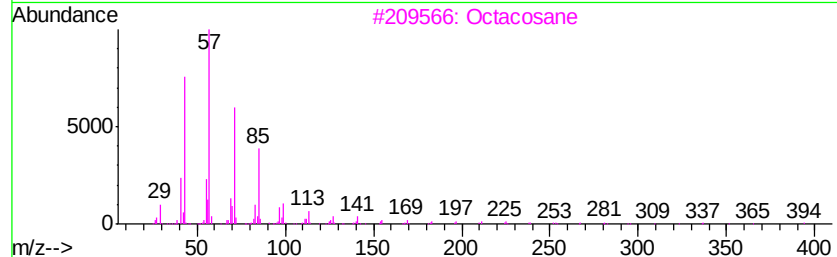
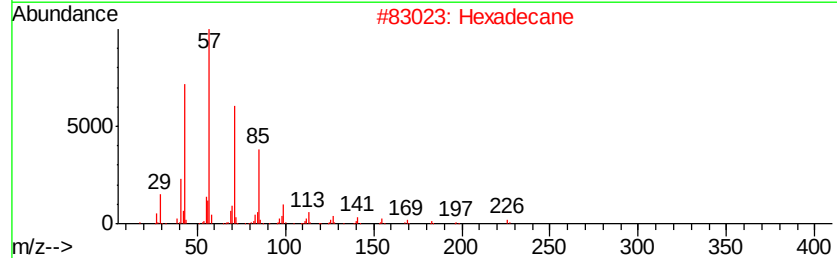
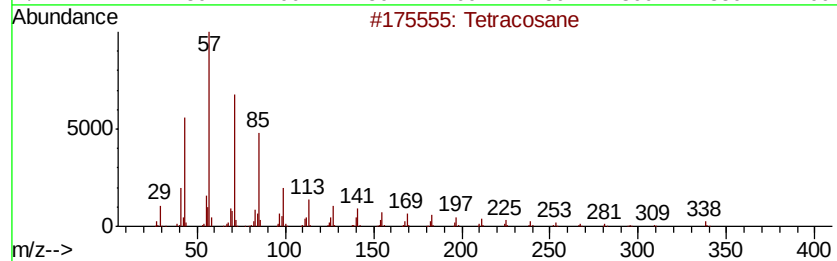
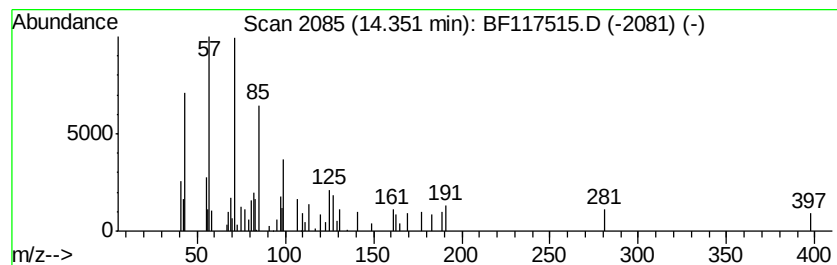
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.28 ng	30764	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	53
2		Hexadecane	226	C16H34	000544-76-3	50
3		Octacosane	394	C28H58	000630-02-4	47
4		Dodecane, 1-iodo-	296	C12H25I	004292-19-7	47
5		Eicosane	282	C20H42	000112-95-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
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Acq On : 24 Oct 2019 17:33
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ClientSampleId :
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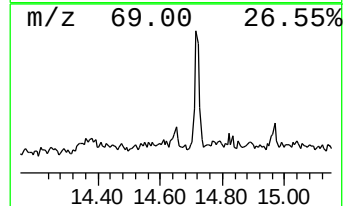
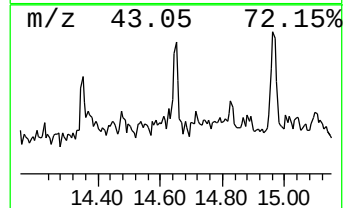
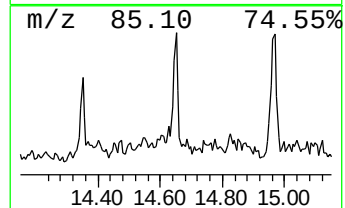
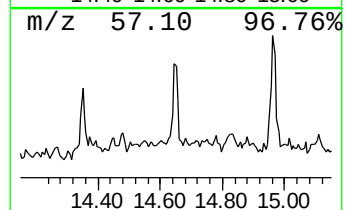
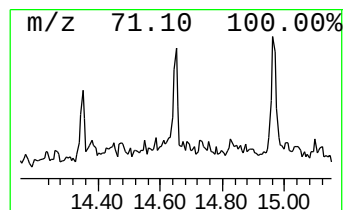
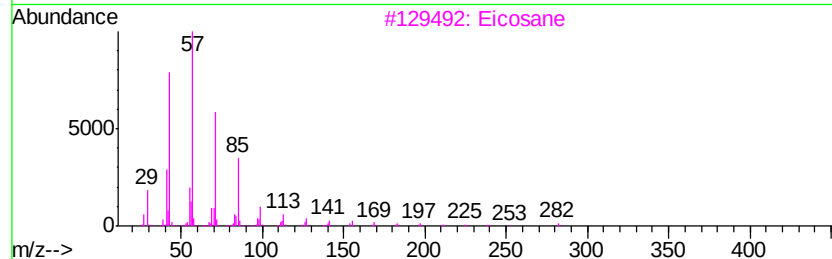
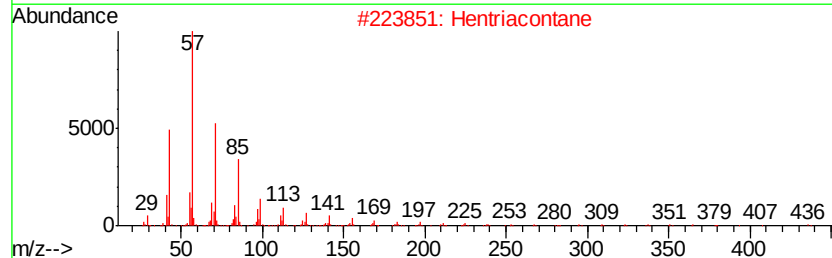
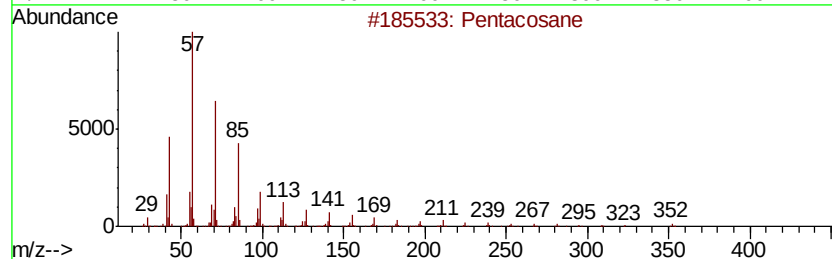
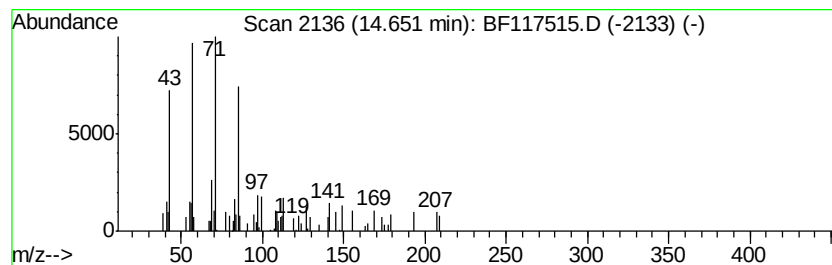
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.65	2.10 ng	36878	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	72
2	Hentriacontane		437	C31H64	000630-04-6	64
3	Eicosane		282	C20H42	000112-95-8	64
4	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	64
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117515.D
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Misc :
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ClientSampleId :
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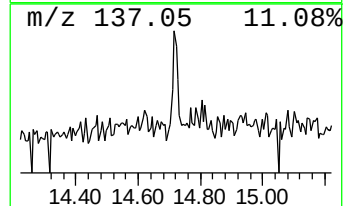
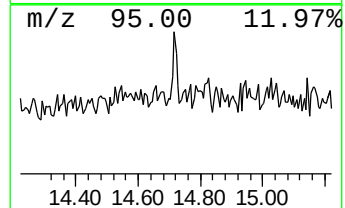
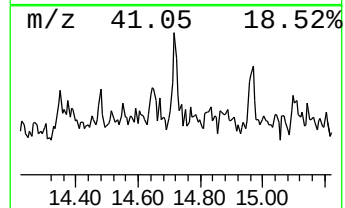
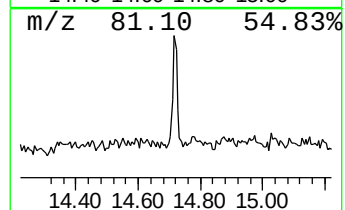
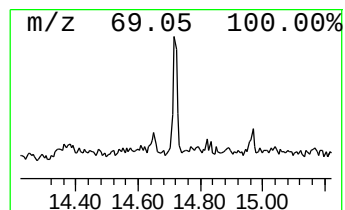
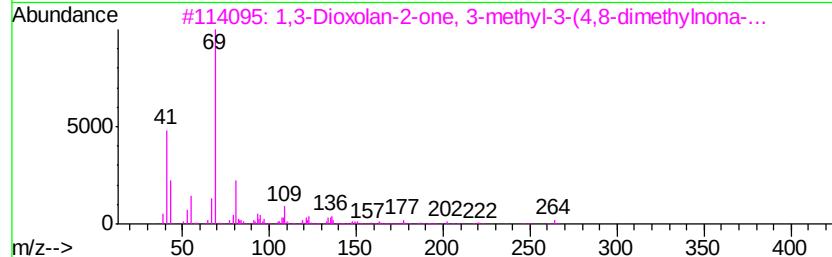
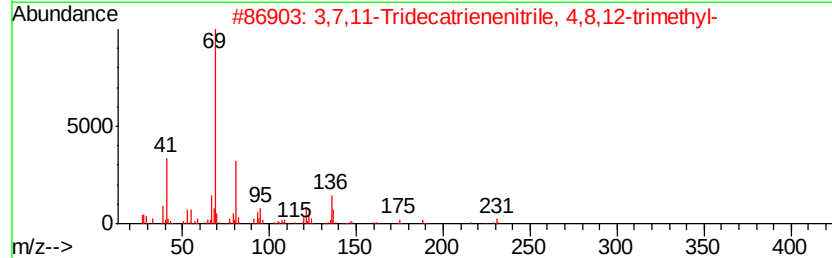
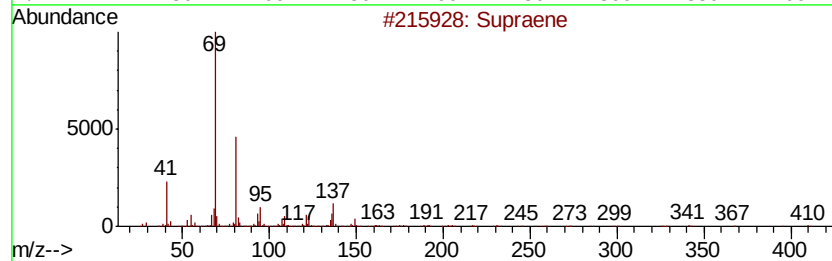
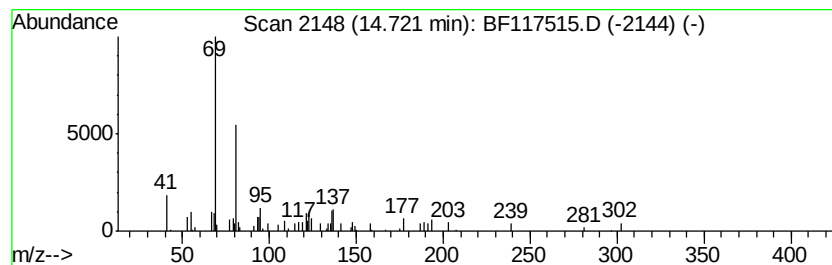
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	2.13 ng	37392	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	59
2		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	53
3		1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	50
4		Squalene	410	C30H50	000111-02-4	50
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117515.D
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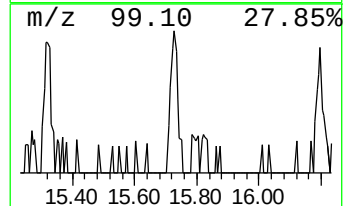
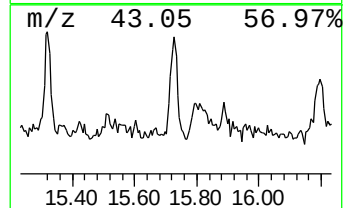
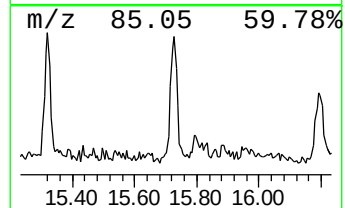
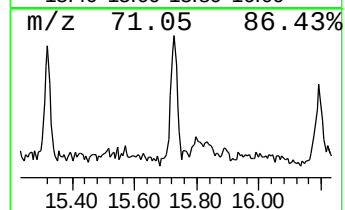
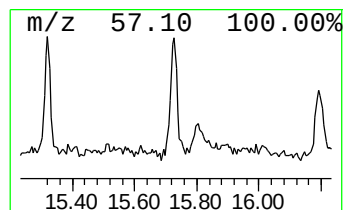
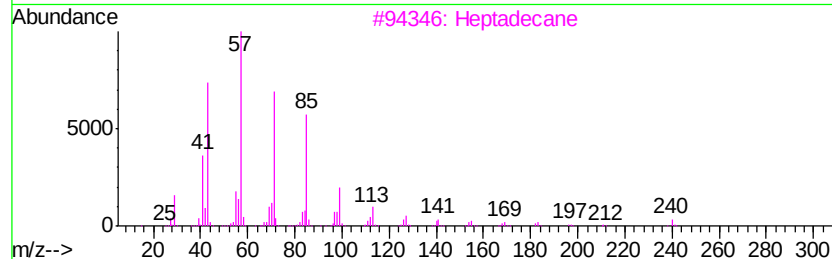
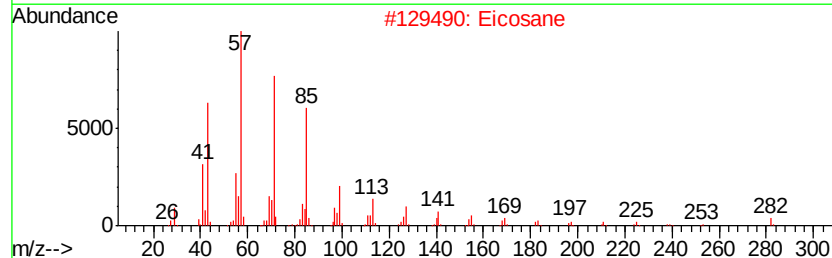
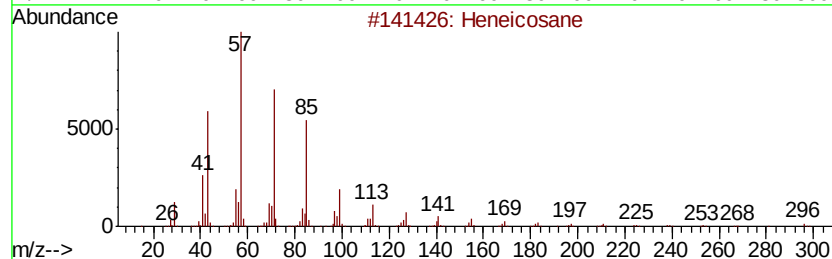
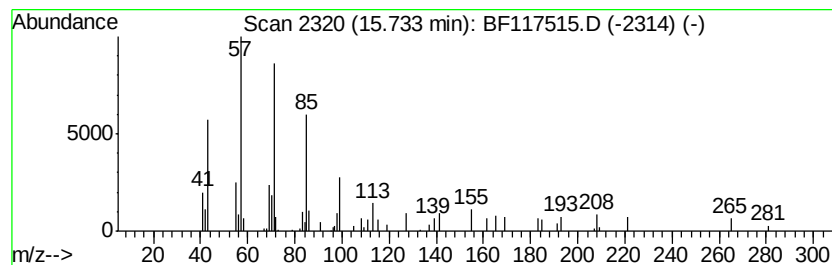
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	3.10 ng	54473	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	83
2		Eicosane	282	C20H42	000112-95-8	80
3		Heptadecane	240	C17H36	000629-78-7	80
4		Triacontane	422	C30H62	000638-68-6	80
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
Data File : BF117515.D
Acq On : 24 Oct 2019 17:33
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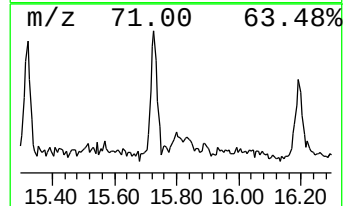
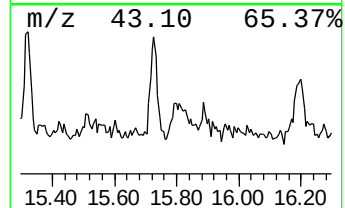
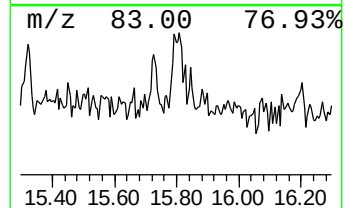
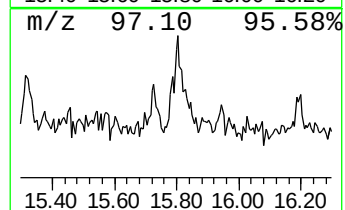
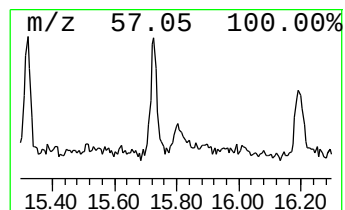
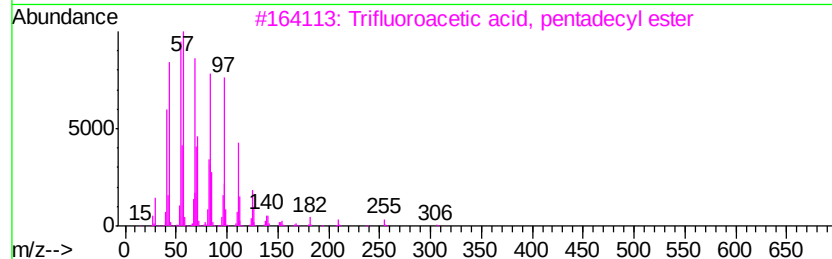
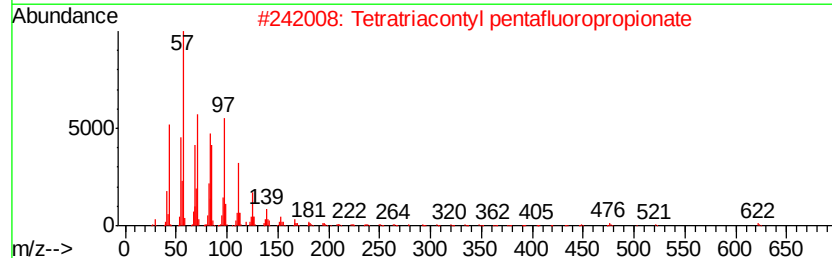
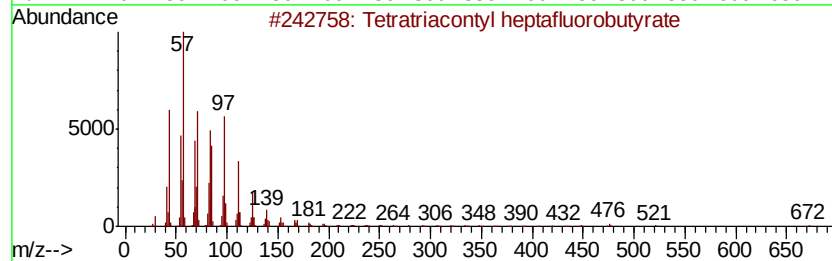
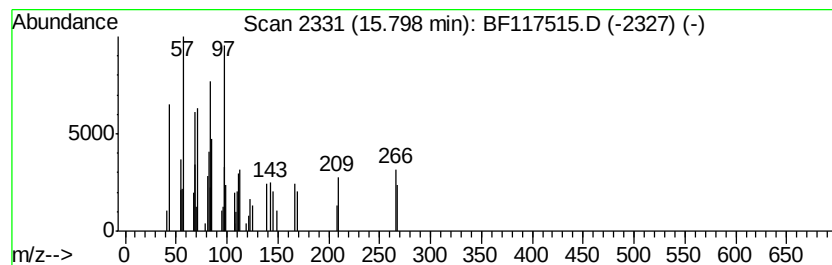
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.80 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.16 ng	55457	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	38
2		Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	35
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	25
4		1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	003731-38-2	22
5		1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102419\
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Acq On : 24 Oct 2019 17:33
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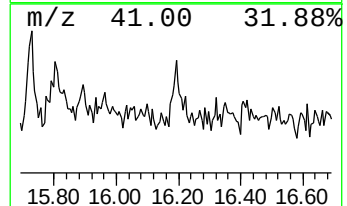
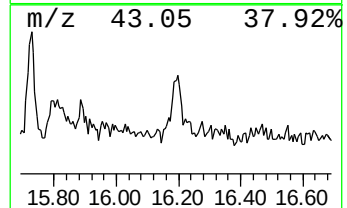
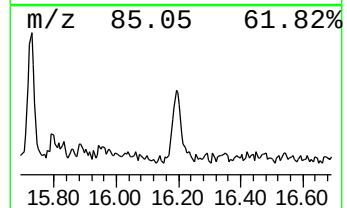
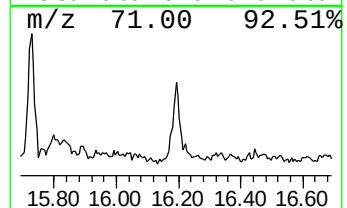
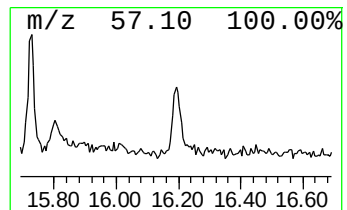
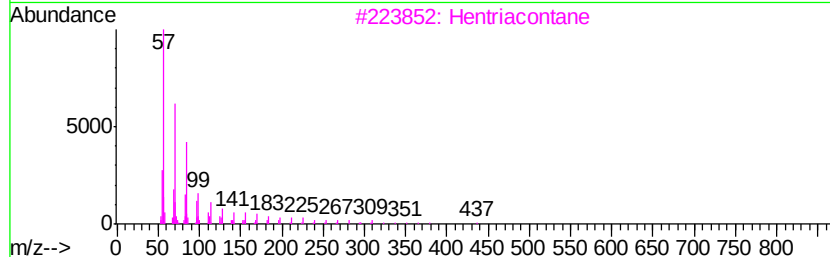
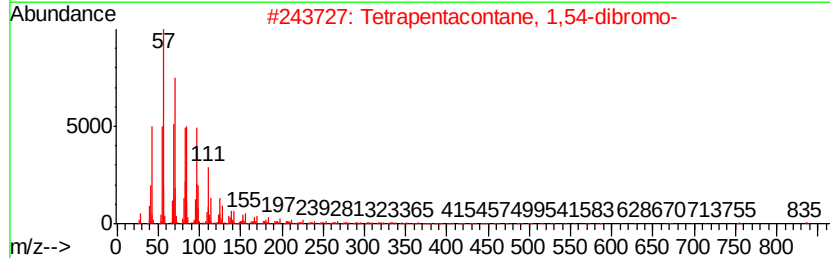
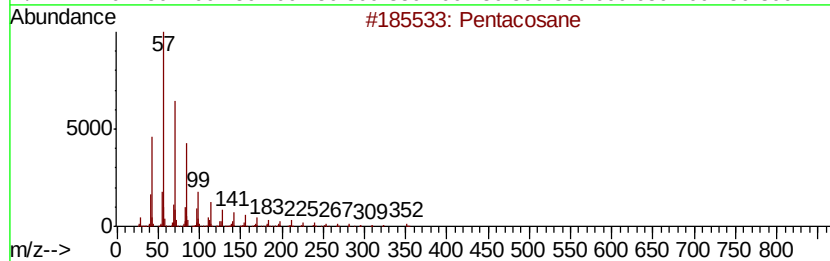
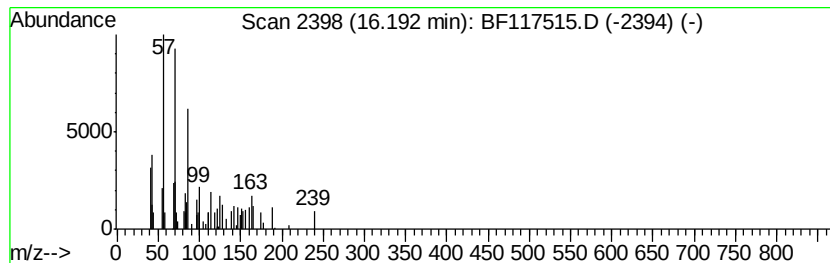
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tridecanol, 2-ethyl-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	2.28 ng	40135	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	64
2		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	64
3		Hentriacontane	437	C31H64	000630-04-6	64
4		Hexacosane	366	C26H54	000630-01-3	64
5		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF102419\
 Data File : BF117515.D
 Acq On : 24 Oct 2019 17:33
 Operator : JU
 Sample : K5499-07
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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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unknown4.94	4.94	2.3	ng	31088	1	6.73	268382	20.0
unknown6.51	6.51	74.3	ng	997746	1	6.73	268382	20.0
n-Hexadecanoic acid	11.78	4.2	ng	76490	4	11.25	366803	20.0
Trichloroacetic a...	13.73	12.1	ng	162524	5	13.89	269690	20.0
Tetracosane	14.35	2.3	ng	30764	5	13.89	269690	20.0
Pentacosane	14.65	2.1	ng	36878	6	15.33	351466	20.0
Supraene	14.72	2.1	ng	37392	6	15.33	351466	20.0
Heneicosane	15.73	3.1	ng	54473	6	15.33	351466	20.0
unknown15.80	15.80	3.2	ng	55457	6	15.33	351466	20.0
Tridecanol, 2-eth...	16.19	2.3	ng	40135	6	15.33	351466	20.0