

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
 Data File : BF118611.D
 Acq On : 21 Jan 2020 00:35
 Operator : CG/JU
 Sample : L1164-06
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 QVD-SB-01-0-52

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-BF012020.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	2.216	13	22	28	rBV	2408269	3284695	31.05%	3.046%
2	5.104	505	513	520	rBV	1551655	2114968	19.99%	1.961%
3	5.504	576	581	584	rBV	8956693	9489637	89.70%	8.800%
4	6.504	745	751	754	rBV	8723906	9951816	94.07%	9.228%
5	6.651	771	776	779	rBV	10295626	10133362	95.78%	9.396%
6	6.881	811	815	818	rBV	3606178	2885759	27.28%	2.676%
7	7.040	837	842	845	rBV	9400300	8144295	76.98%	7.552%
8	7.440	904	910	913	rBV	6178839	6111497	57.77%	5.667%
9	8.163	1028	1033	1036	rBV	4024861	3455365	32.66%	3.204%
10	9.239	1210	1216	1219	rBV	11754995	10579431	100.00%	9.810%
11	9.628	1279	1282	1285	rBV	621655	485530	4.59%	0.450%
12	9.916	1325	1331	1334	rBV	3949460	3398113	32.12%	3.151%
13	9.951	1334	1337	1340	rVB	127803	123133	1.16%	0.114%
14	10.463	1421	1424	1427	rBV	144253	122425	1.16%	0.114%
15	10.704	1460	1465	1468	rBV	6320569	5622534	53.15%	5.214%
16	10.828	1483	1486	1488	rBV	115873	116993	1.11%	0.108%
17	11.404	1580	1584	1586	rBV	3124808	2975129	28.12%	2.759%
18	11.428	1586	1588	1591	rVV	1382226	1101016	10.41%	1.021%
19	11.475	1591	1596	1599	rVB	412052	380392	3.60%	0.353%
20	11.622	1617	1621	1625	rBV2	104474	123042	1.16%	0.114%
21	11.927	1670	1673	1678	rVB	625179	522047	4.93%	0.484%
22	12.016	1684	1688	1690	rBV2	232528	222869	2.11%	0.207%
23	12.498	1765	1770	1774	rBV5	118033	230212	2.18%	0.213%
24	12.610	1786	1789	1793	rBV	1810817	1635759	15.46%	1.517%
25	12.710	1803	1806	1812	rBV6	139967	211848	2.00%	0.196%
26	12.839	1823	1828	1831	rBV	1538113	1590611	15.03%	1.475%
27	12.986	1849	1853	1856	rBV	9995893	8569926	81.01%	7.947%
28	13.169	1882	1884	1887	rVB	188406	157835	1.49%	0.146%
29	13.233	1891	1895	1898	rVV2	206097	272040	2.57%	0.252%
30	13.469	1933	1935	1941	rVB2	121077	137337	1.30%	0.127%
31	13.569	1949	1952	1954	rBV	218769	203734	1.93%	0.189%
32	13.880	2002	2005	2015	rVB2	1372677	1565486	14.80%	1.452%
33	14.039	2027	2032	2034	rBV2	3317588	3650836	34.51%	3.385%
34	14.063	2034	2036	2039	rVB	705579	532503	5.03%	0.494%

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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	14.210	2059	2061	2066	rVB2	503923	482585	4.56%	0.447%
36	14.516	2110	2113	2116	rBV	810063	727190	6.87%	0.674%
37	14.827	2163	2166	2169	rBV	726673	711296	6.72%	0.660%
38	15.080	2206	2209	2219	rVB	631537	1293699	12.23%	1.200%
39	15.168	2221	2224	2235	rVB2	764139	1082645	10.23%	1.004%
40	15.386	2258	2261	2267	rVB	356476	429430	4.06%	0.398%
41	15.445	2268	2271	2277	rBV	430714	508611	4.81%	0.472%
42	15.510	2278	2282	2286	rBV	1790001	2166756	20.48%	2.009%
43	15.998	2363	2365	2370	rVB	308192	337517	3.19%	0.313%

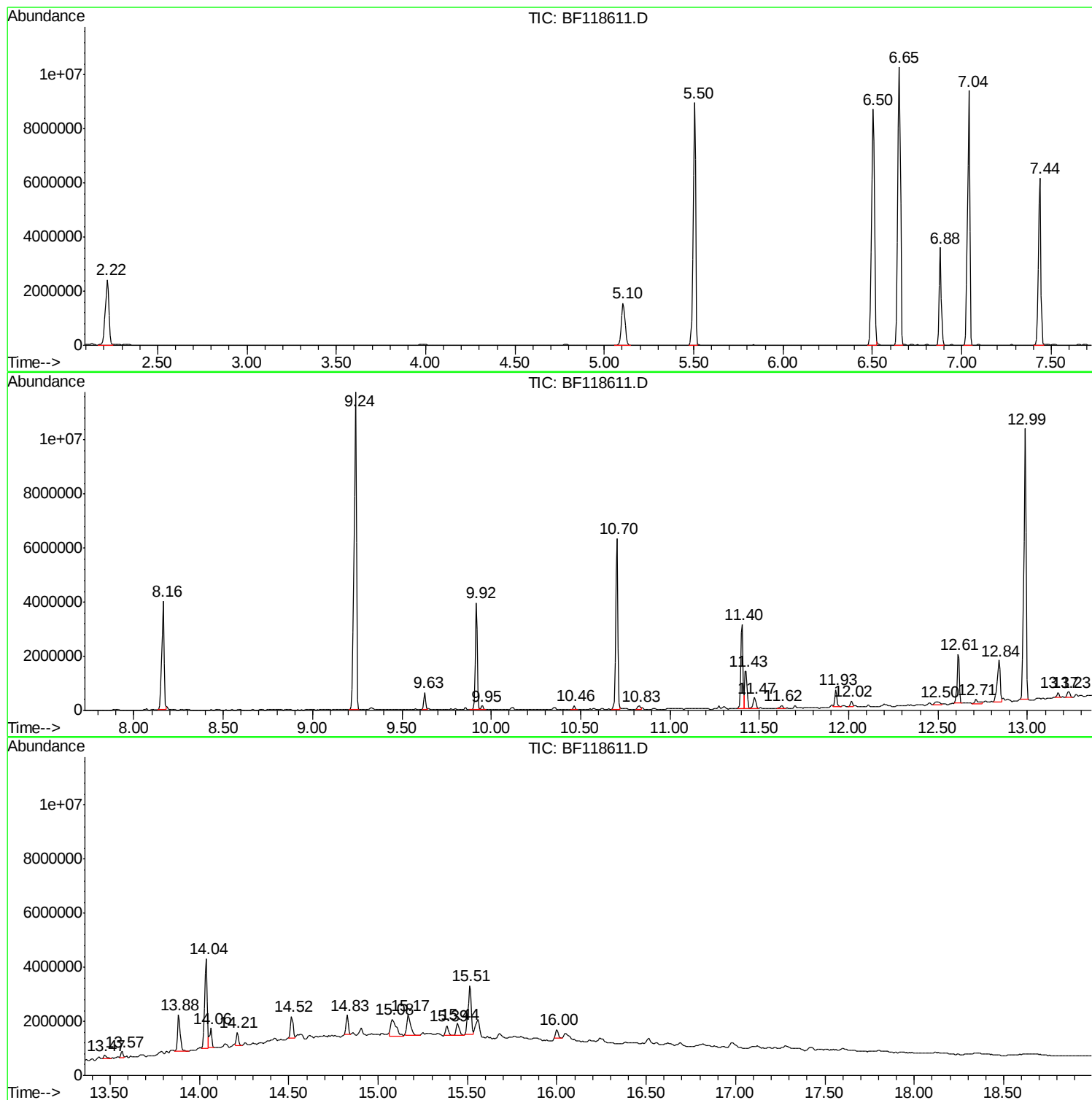
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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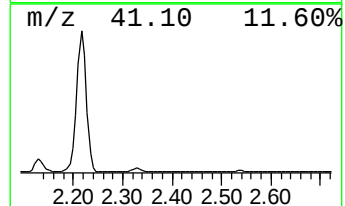
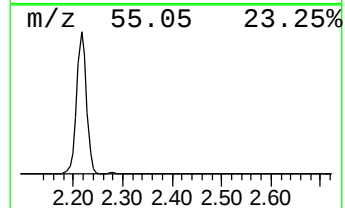
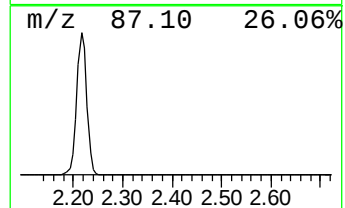
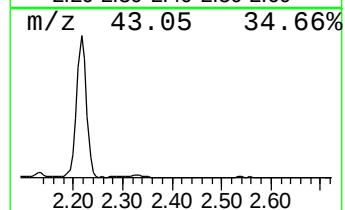
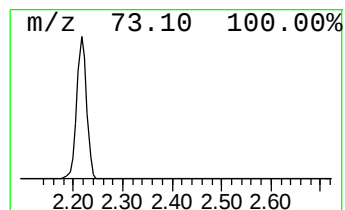
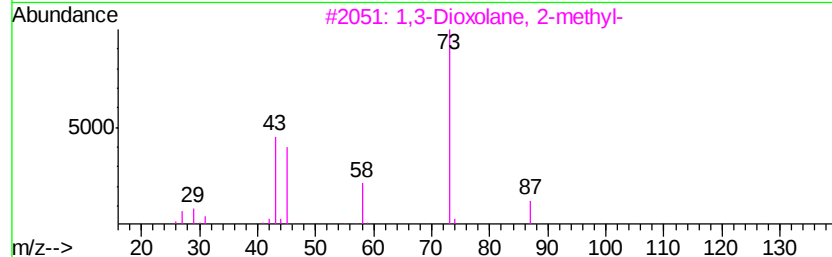
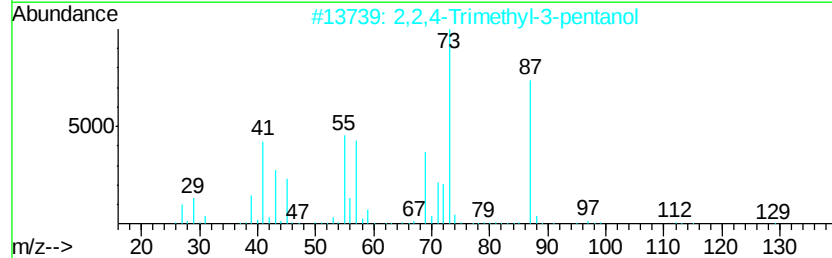
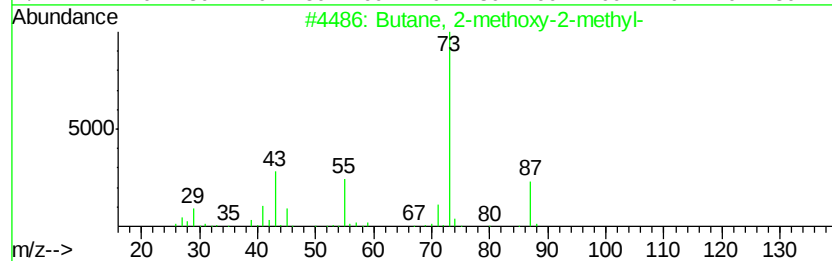
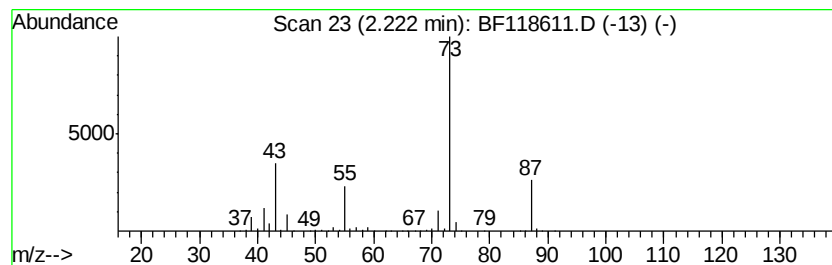
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	22.76 ng	3284700	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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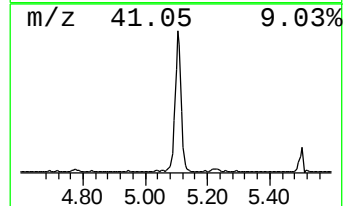
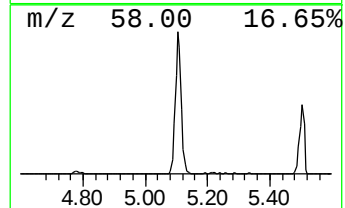
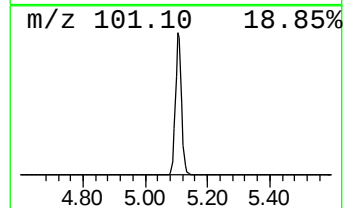
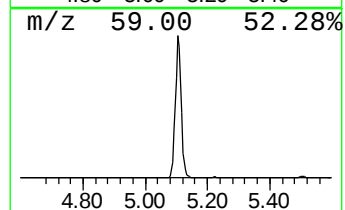
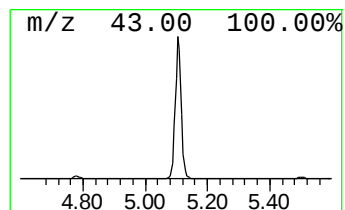
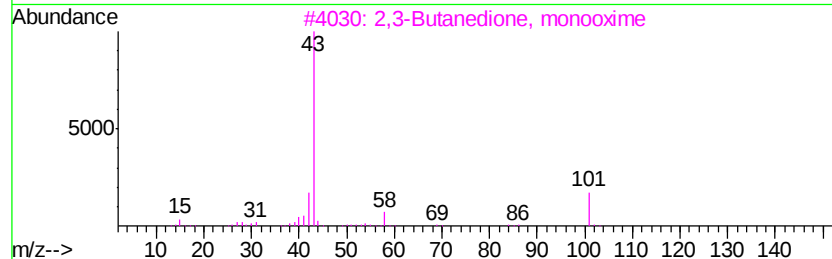
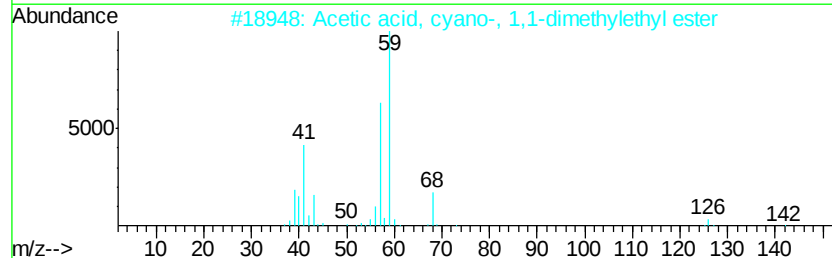
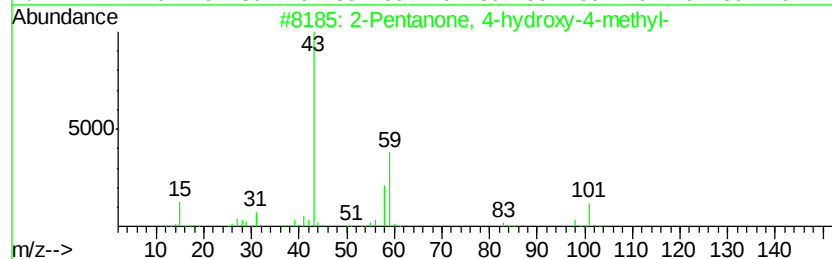
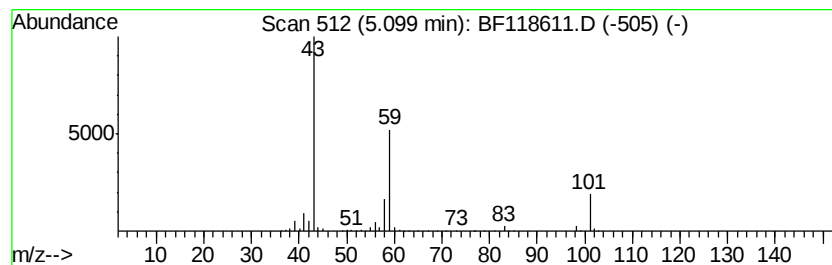
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	14.66 ng	2114970	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4		Acetone	58	C3H6O	000067-64-1	10
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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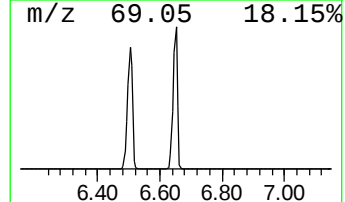
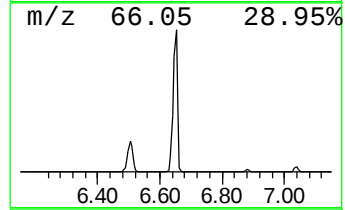
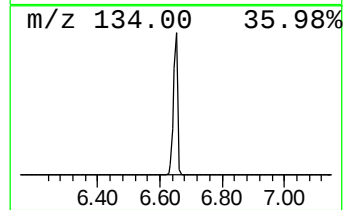
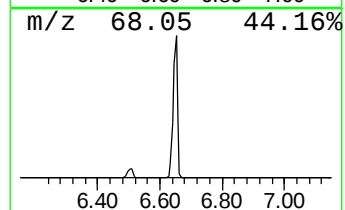
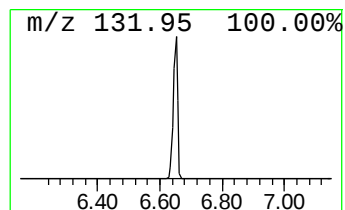
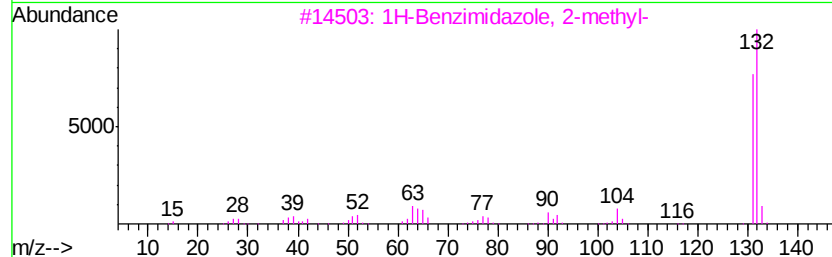
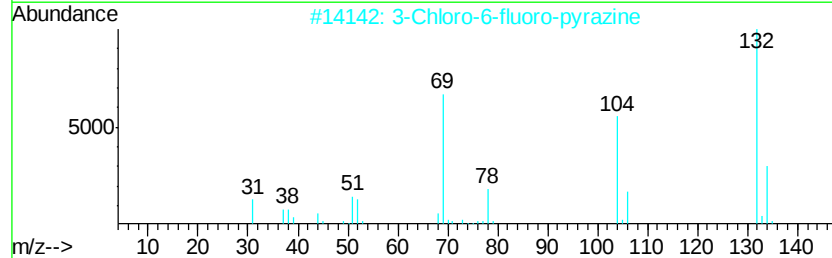
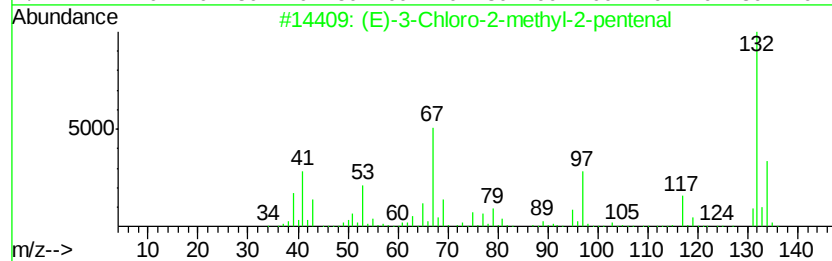
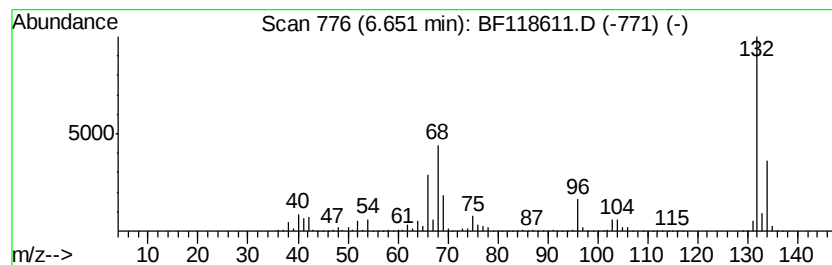
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.23 ng	10133400	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	12



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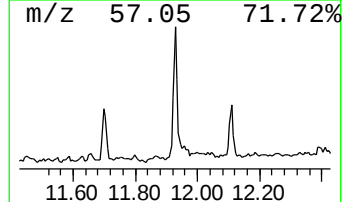
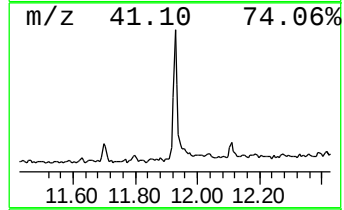
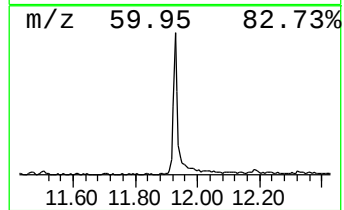
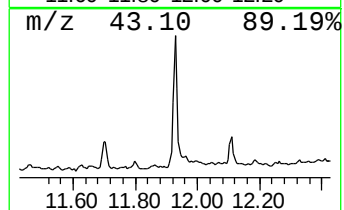
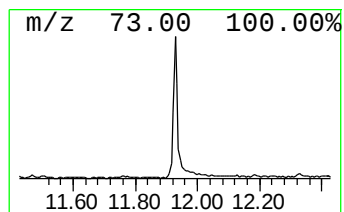
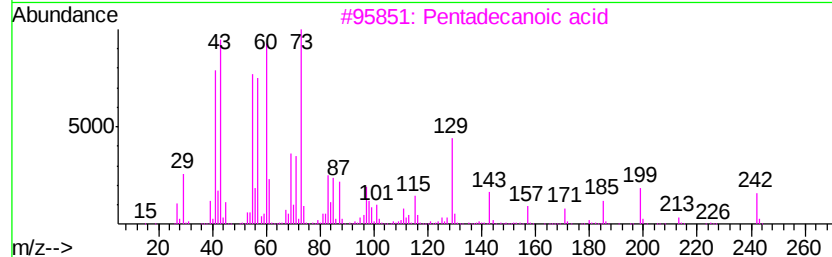
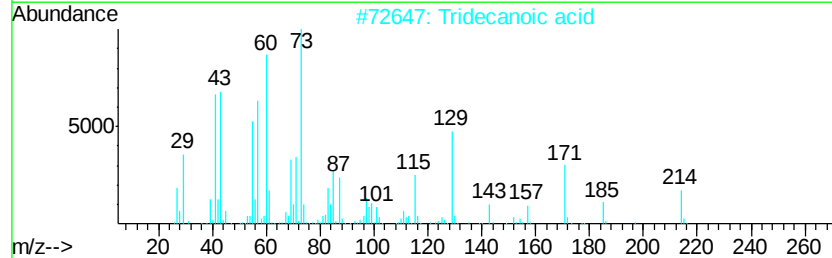
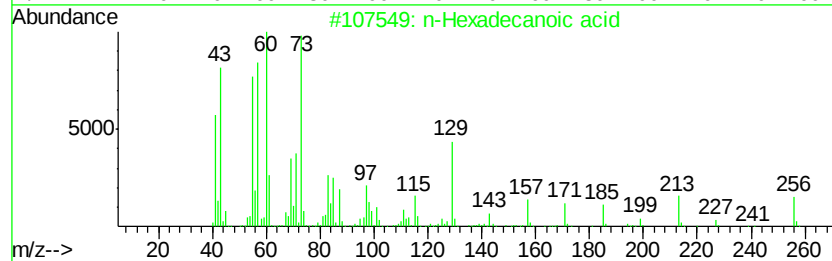
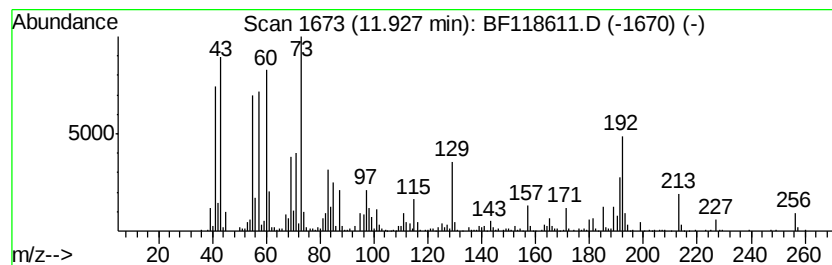
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.51 ng	522047	Phenanthrene-d10	11.40

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	60
5		Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	30



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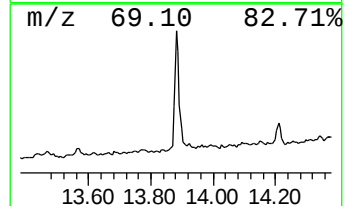
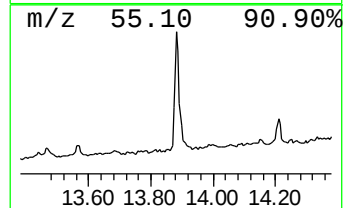
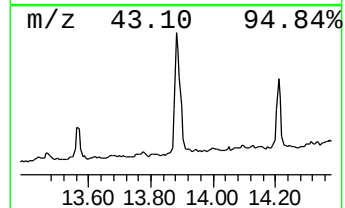
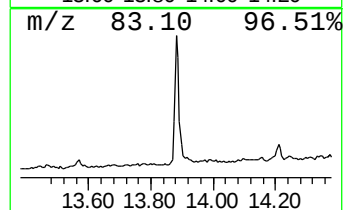
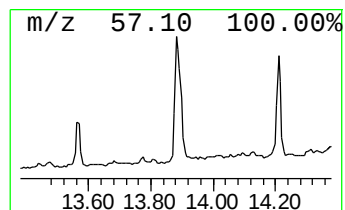
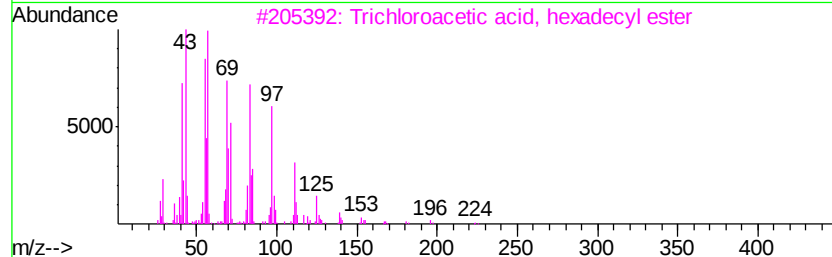
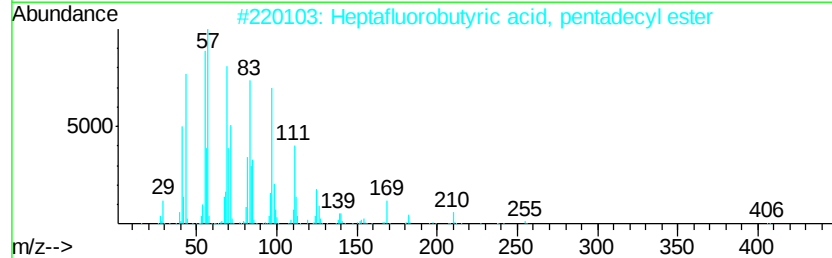
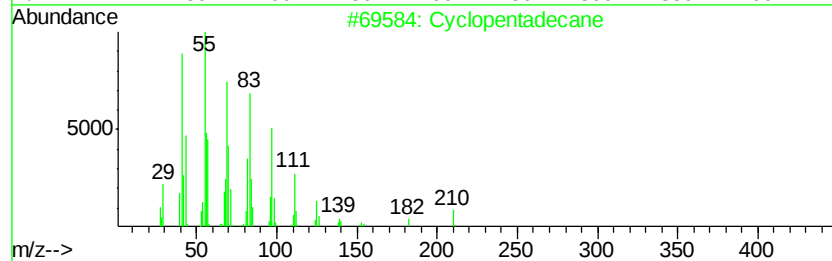
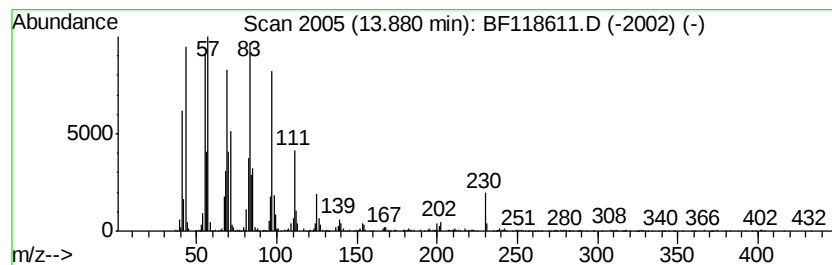
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ClientSampleId :
QVD-SB-01-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.88	8.58 ng	1565490	Chrysene-d12	14.04	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclopentadecane	210	C15H30	000295-48-7	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118611.D
Acq On : 21 Jan 2020 00:35
Operator : CG/JU
Sample : L1164-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

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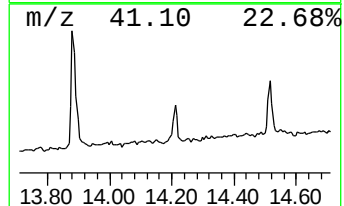
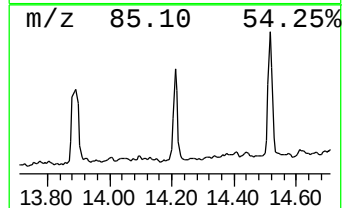
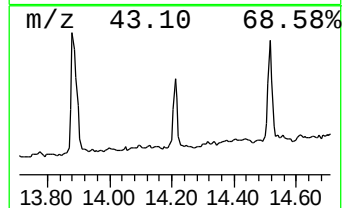
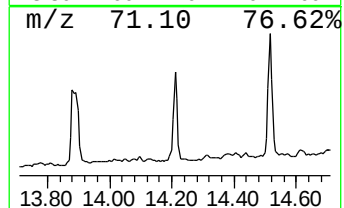
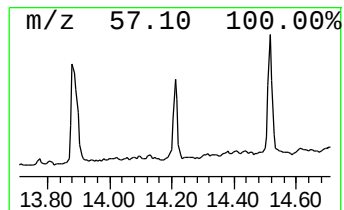
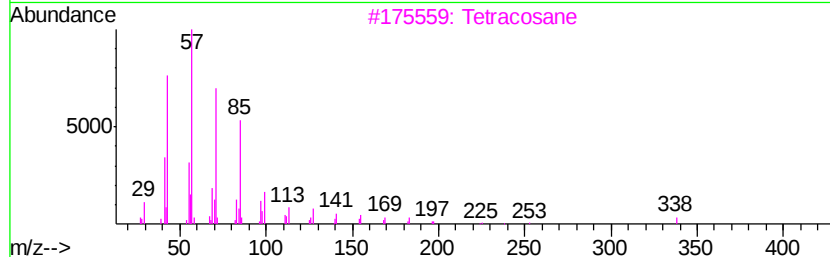
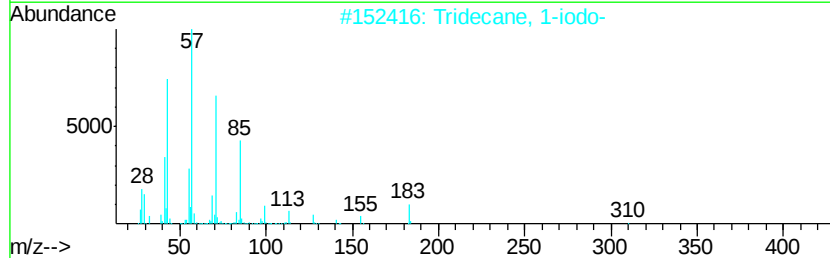
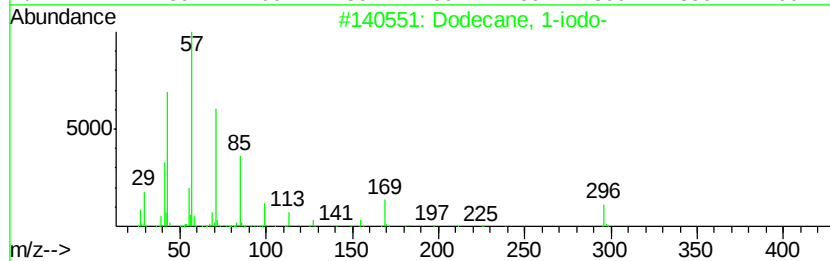
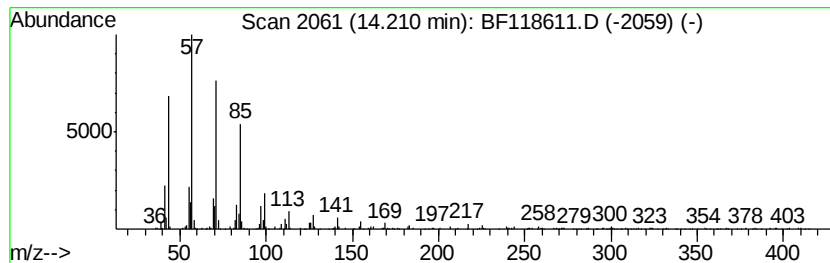
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dodecane, 1-iodo- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.64 ng	482585	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	93
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3		Tetracosane	338	C24H50	000646-31-1	91
4		Hexadecane	226	C16H34	000544-76-3	91
5		Docosane, 11-butyl-	366	C26H54	013475-76-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118611.D
Acq On : 21 Jan 2020 00:35
Operator : CG/JU
Sample : L1164-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
QVD-SB-01-0-52

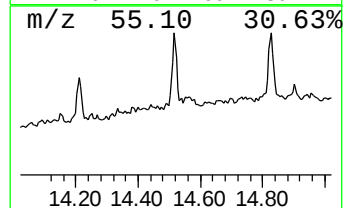
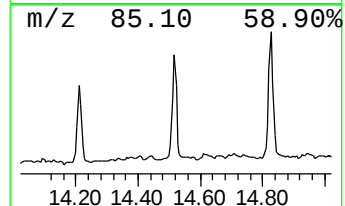
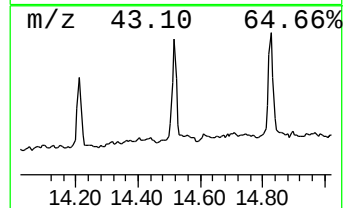
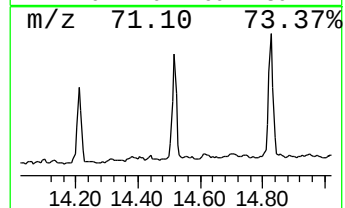
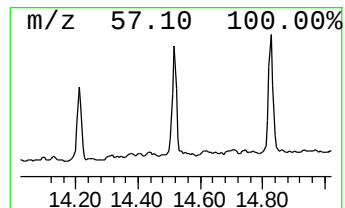
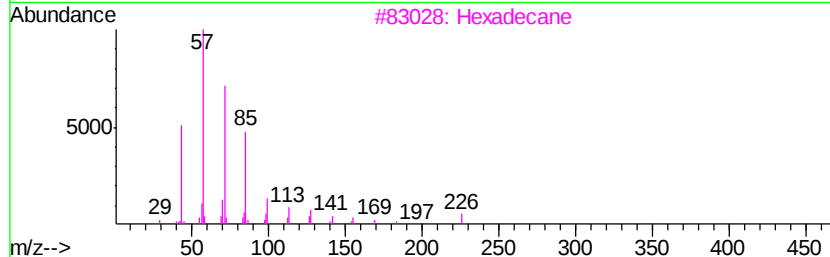
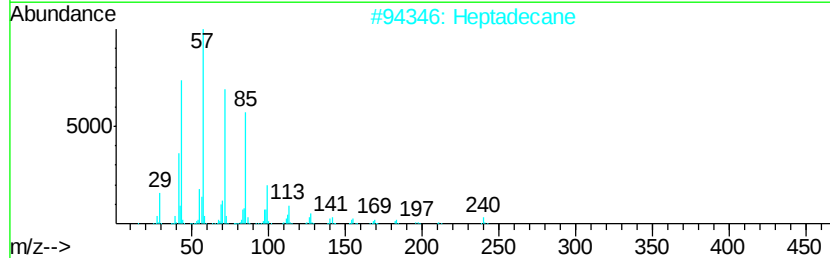
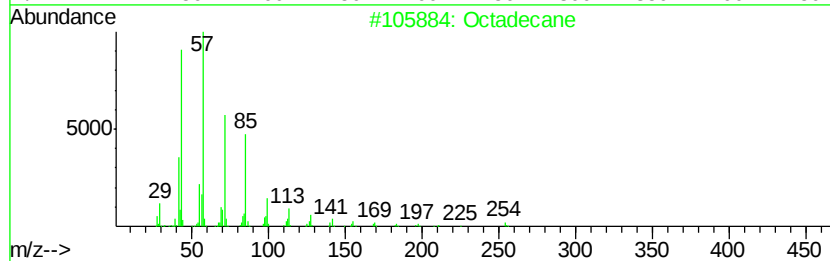
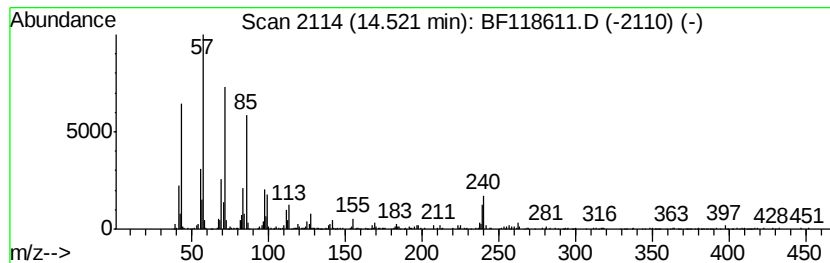
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	3.98 ng	727190	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Heptadecane	240	C17H36	000629-78-7	94
3		Hexadecane	226	C16H34	000544-76-3	91
4		Eicosane, 9-octyl-	394	C28H58	013475-77-9	91
5		2-Bromo dodecane	248	C12H25Br	013187-99-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118611.D
Acq On : 21 Jan 2020 00:35
Operator : CG/JU
Sample : L1164-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

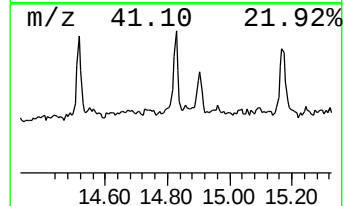
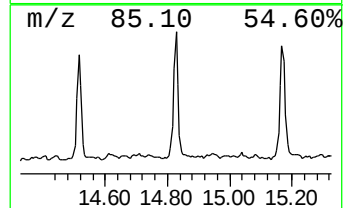
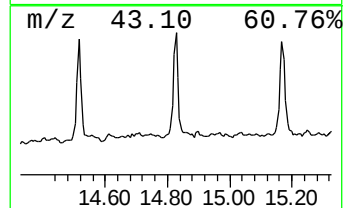
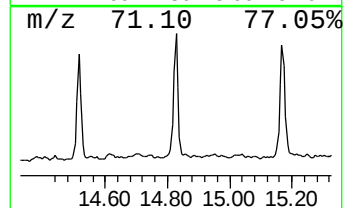
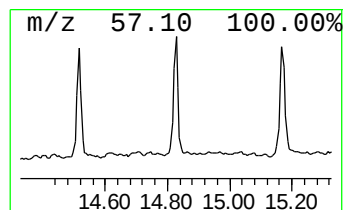
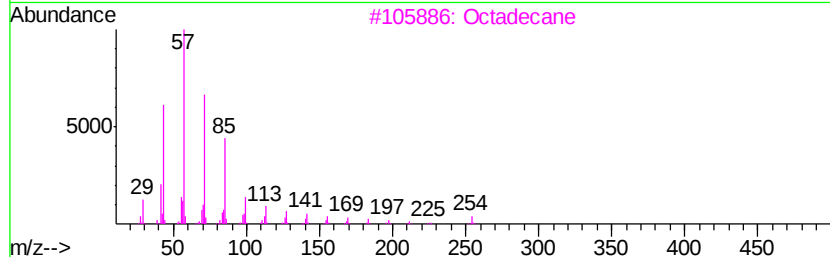
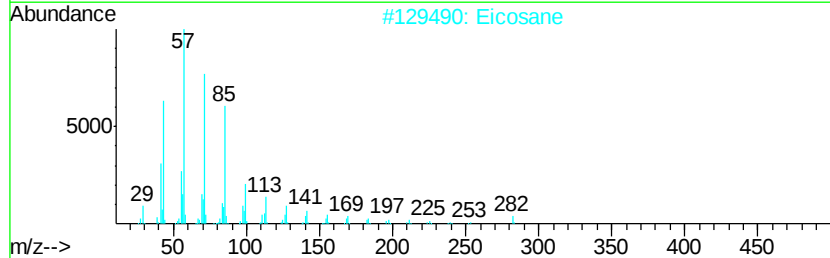
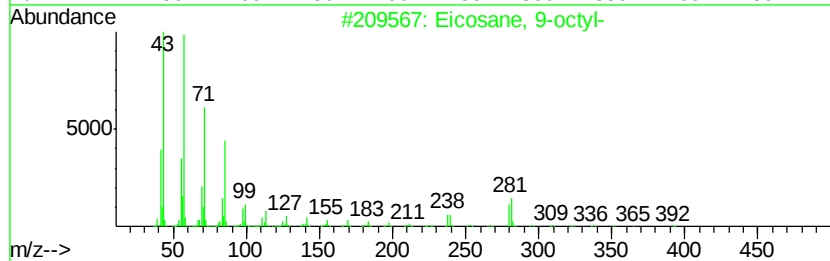
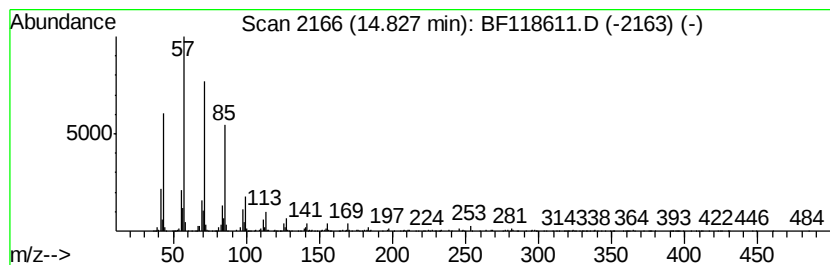
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane, 9-octyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.83	6.57 ng	711296	Perylene-d12	15.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 9-octyl-	394	C28H58	013475-77-9	94
2	Eicosane	282	C20H42	000112-95-8	94
3	Octadecane	254	C18H38	000593-45-3	93
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tetracosane	338	C24H50	000646-31-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118611.D
Acq On : 21 Jan 2020 00:35
Operator : CG/JU
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Misc :
ALS Vial : 21 Sample Multiplier: 1

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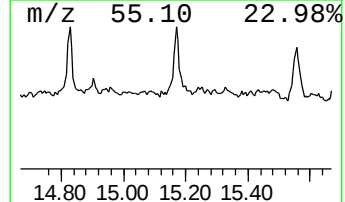
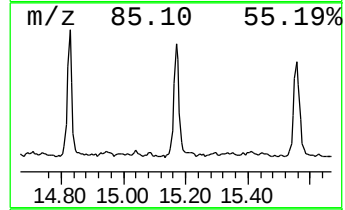
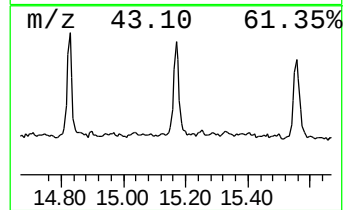
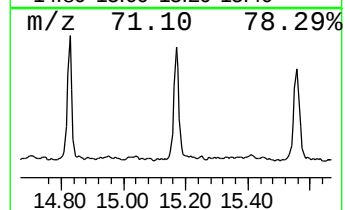
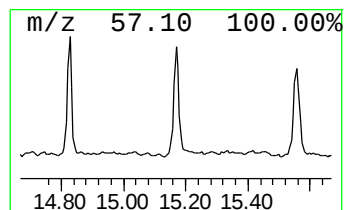
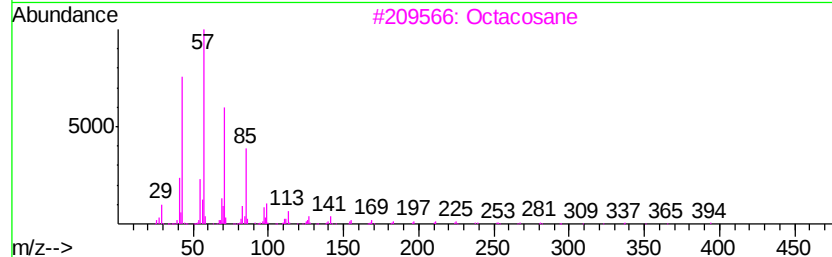
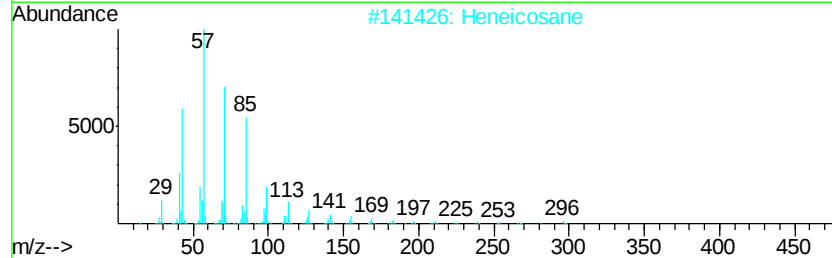
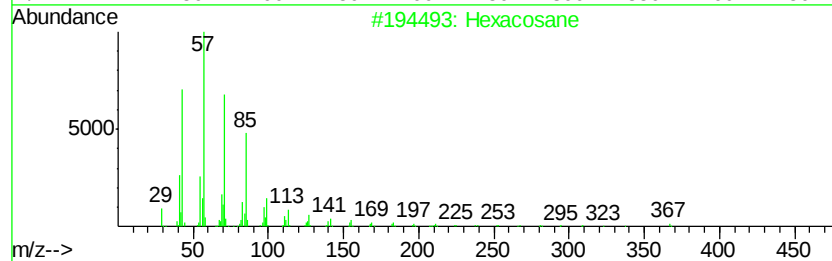
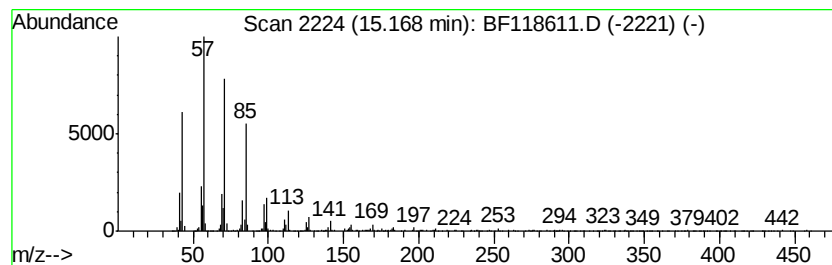
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	9.99 ng	1082650	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		2-methyloctacosane	408	C29H60	1000376-72-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118611.D
Acq On : 21 Jan 2020 00:35
Operator : CG/JU
Sample : L1164-06
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
QVD-SB-01-0-52

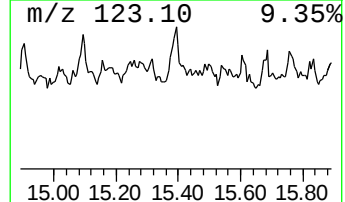
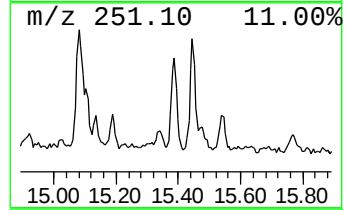
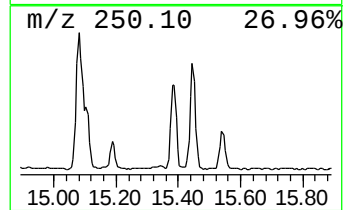
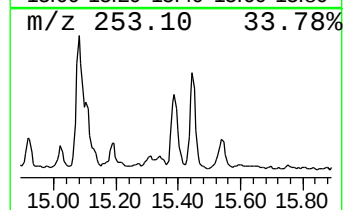
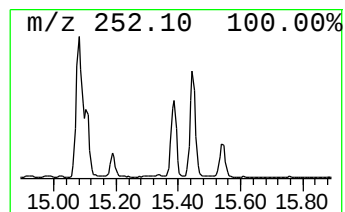
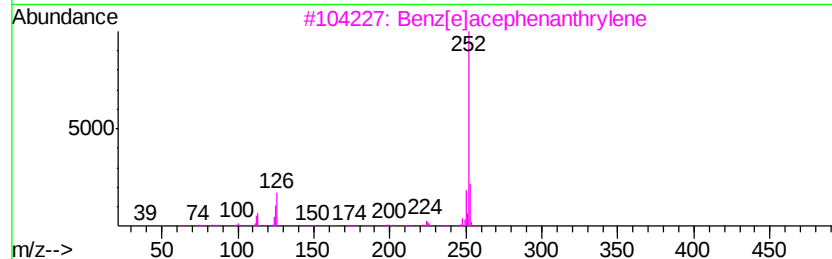
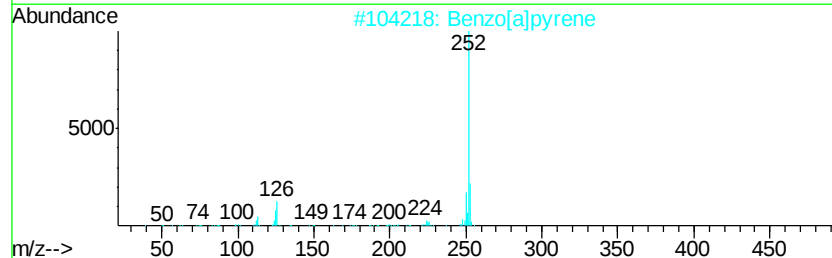
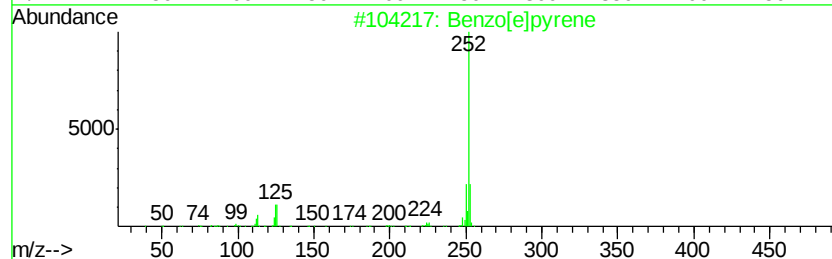
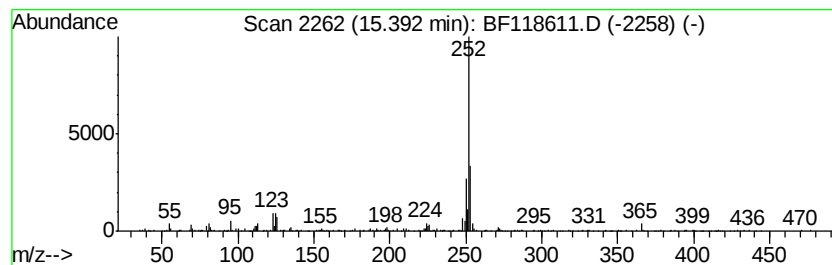
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	3.96 ng	429430	Perylene-d12	15.51

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[a]pyrene	252	C20H12	000050-32-8	93
3			Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	93
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	92
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
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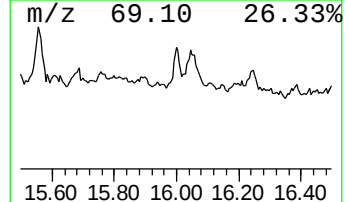
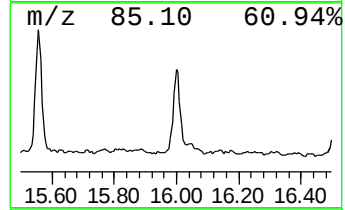
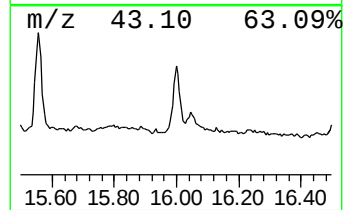
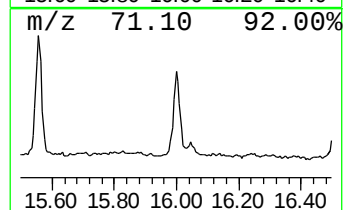
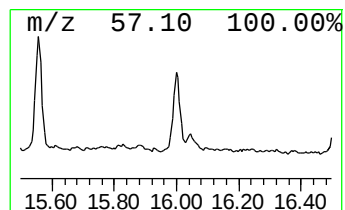
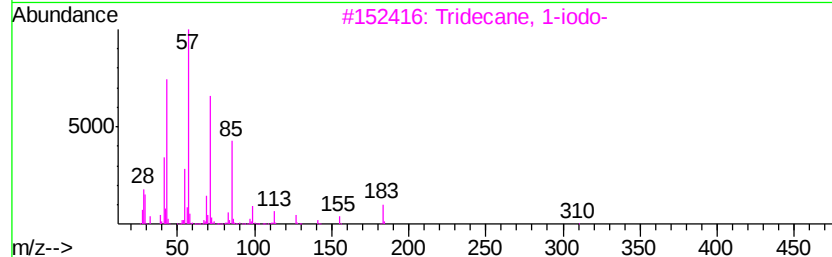
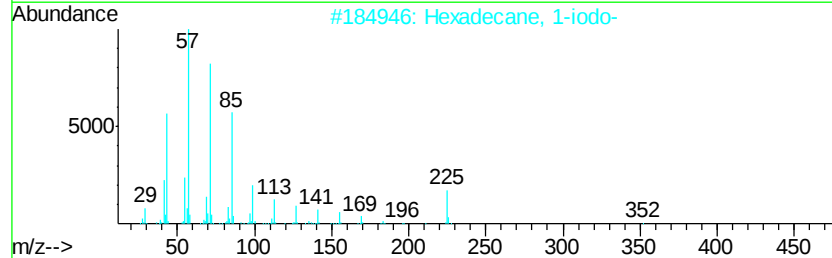
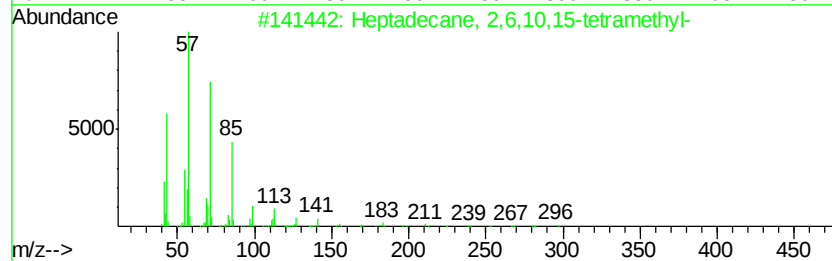
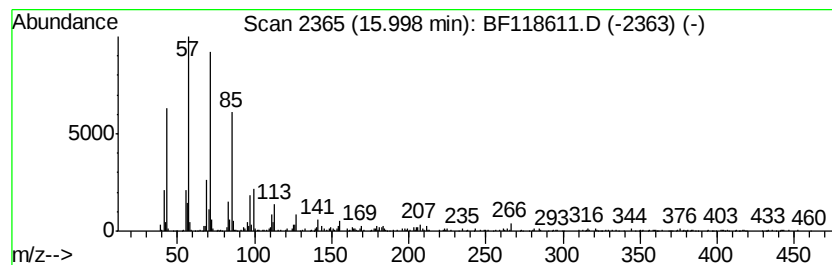
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptadecane, 2,6,10,15-tetr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	3.12 ng	337517	Perylene-d12	15.51

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	89
4		Tetracosane	338	C24H50	000646-31-1	87
5		Octadecane, 2,6,10,14-tetramethyl-	310	C22H46	054964-82-8	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
QVD-SB-01-0-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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2-Pentanone, 4-hy...	5.10	14.7	ng	2114970	1	6.88	2885760	20.0
unknown6.65	6.65	70.2	ng	10133400	1	6.88	2885760	20.0
n-Hexadecanoic acid	11.93	3.5	ng	522047	4	11.40	2975130	20.0
Cyclopentadecane	13.88	8.6	ng	1565490	5	14.04	3650840	20.0
Dodecane, 1-iodo-	14.21	2.6	ng	482585	5	14.04	3650840	20.0
Octadecane	14.52	4.0	ng	727190	5	14.04	3650840	20.0
Eicosane, 9-octyl-	14.83	6.6	ng	711296	6	15.51	2166760	20.0
Hexacosane	15.17	10.0	ng	1082650	6	15.51	2166760	20.0
Benzo[e]pyrene	15.39	4.0	ng	429430	6	15.51	2166760	20.0
Heptadecane, 2,6,...	16.00	3.1	ng	337517	6	15.51	2166760	20.0