

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
 Data File : BF118391.D
 Acq On : 30 Dec 2019 20:01
 Operator : JU
 Sample : K6455-06
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 K435-WC-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-BF122419.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	521	rVB	438625	572031	14.40%	1.449%
2	5.475	572	576	598	rBV	2767673	2700884	67.97%	6.843%
3	6.492	744	749	767	rBV	2999381	3011567	75.79%	7.631%
4	6.628	767	772	775	rBV	3383553	3215266	80.92%	8.147%
5	6.851	806	810	815	rBV	967377	782102	19.68%	1.982%
6	7.010	831	837	840	rBV2	3182936	3346722	84.23%	8.480%
7	7.416	902	906	918	rBV	1750223	1902943	47.89%	4.822%
8	8.139	1025	1029	1041	rVB	1087882	1013779	25.51%	2.569%
9	9.216	1208	1212	1215	rBV	4740813	3973414	100.00%	10.068%
10	9.292	1222	1225	1228	rVB	84357	71267	1.79%	0.181%
11	9.486	1254	1258	1262	rBV	55674	67170	1.69%	0.170%
12	9.610	1276	1279	1288	rVB	247160	274139	6.90%	0.695%
13	9.822	1310	1315	1319	rBV	99741	87617	2.21%	0.222%
14	9.898	1320	1328	1332	rBV	1387851	1230506	30.97%	3.118%
15	9.927	1332	1333	1337	rVB	54624	48507	1.22%	0.123%
16	10.104	1361	1363	1367	rVB4	43341	51078	1.29%	0.129%
17	10.145	1367	1370	1374	rVB3	50185	53850	1.36%	0.136%
18	10.216	1379	1382	1385	rBV2	38936	46558	1.17%	0.118%
19	10.322	1397	1400	1403	rVB	129502	110590	2.78%	0.280%
20	10.451	1417	1422	1427	rBV5	35160	63182	1.59%	0.160%
21	10.545	1434	1438	1444	rVB2	60184	94438	2.38%	0.239%
22	10.698	1460	1464	1473	rBV	2040232	2154259	54.22%	5.458%
23	10.798	1478	1481	1482	rBV	137908	120547	3.03%	0.305%
24	11.245	1554	1557	1560	rBV2	124356	113719	2.86%	0.288%
25	11.280	1560	1563	1569	rVB3	74310	107467	2.70%	0.272%
26	11.392	1579	1582	1585	rBV	1306831	1230276	30.96%	3.117%
27	11.416	1585	1586	1592	rVV	437294	340196	8.56%	0.862%
28	11.469	1592	1595	1598	rVB	58483	73339	1.85%	0.186%
29	11.627	1618	1622	1627	rBV3	44738	71956	1.81%	0.182%
30	11.674	1627	1630	1634	rVB2	102585	88153	2.22%	0.223%
31	11.916	1665	1671	1678	rBV3	416008	569845	14.34%	1.444%
32	12.010	1684	1687	1689	rBV2	103498	110751	2.79%	0.281%
33	12.033	1689	1691	1694	rVB	75771	61509	1.55%	0.156%
34	12.086	1697	1700	1703	rBV	93970	90260	2.27%	0.229%

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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	12.192	1716	1718	1722	rBV	64848	64292	1.62%	0.163%
36	12.451	1758	1762	1764	rBV	92027	97146	2.44%	0.246%
37	12.474	1764	1766	1770	rVV3	100371	108445	2.73%	0.275%
38	12.539	1774	1777	1781	rBV2	48764	61193	1.54%	0.155%
39	12.616	1786	1790	1794	rBV	631191	628046	15.81%	1.591%
40	12.704	1802	1805	1809	rBV2	123677	145659	3.67%	0.369%
41	12.845	1823	1829	1832	rBV	669737	691182	17.40%	1.751%
42	12.986	1845	1853	1856	rBV	4067076	3661559	92.15%	9.278%
43	13.063	1862	1866	1872	rBV3	49320	101312	2.55%	0.257%
44	13.174	1878	1885	1886	rBV2	69543	118149	2.97%	0.299%
45	13.204	1888	1890	1894	rVB2	86376	84269	2.12%	0.214%
46	13.280	1899	1903	1905	rBV2	72881	78939	1.99%	0.200%
47	13.551	1946	1949	1951	rBV	88545	79222	1.99%	0.201%
48	13.880	2001	2005	2015	rVB2	664721	944358	23.77%	2.393%
49	14.051	2029	2034	2037	rBV2	955764	1122279	28.24%	2.844%
50	14.074	2037	2038	2041	rVB	247799	160771	4.05%	0.407%
51	14.198	2056	2059	2067	rBV	191004	209705	5.28%	0.531%
52	14.504	2108	2111	2119	rBV2	263183	473838	11.93%	1.201%
53	14.815	2161	2164	2167	rVB	238093	239398	6.02%	0.607%
54	15.104	2210	2213	2217	rBV	199466	303477	7.64%	0.769%
55	15.157	2219	2222	2225	rVB	281566	293643	7.39%	0.744%
56	15.415	2263	2266	2272	rVB	134275	166332	4.19%	0.421%
57	15.480	2274	2277	2283	rVV	204968	251996	6.34%	0.639%
58	15.545	2283	2288	2300	rVB	906633	1261506	31.75%	3.196%
59	15.986	2359	2363	2368	rBV	180483	269948	6.79%	0.684%

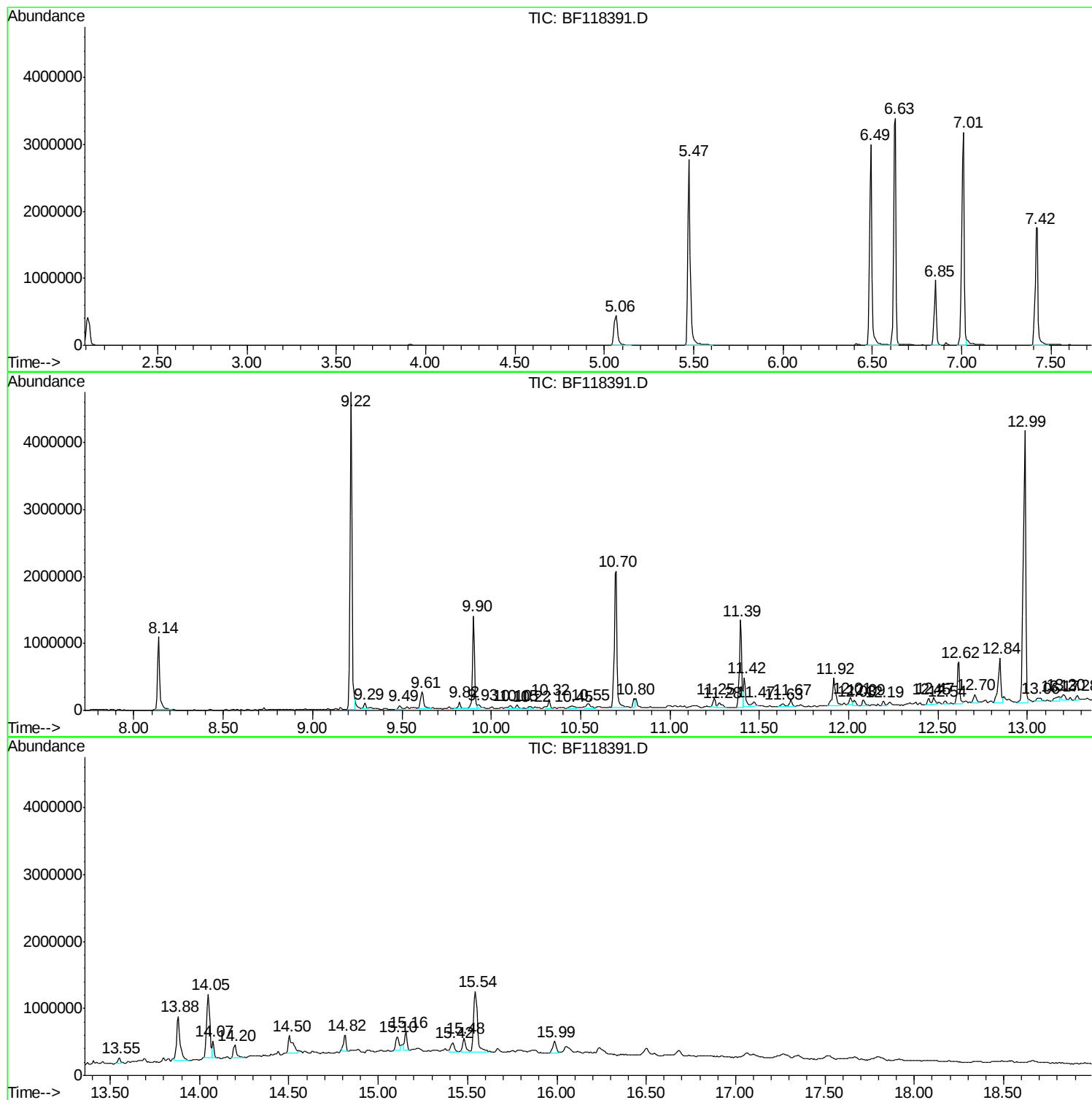
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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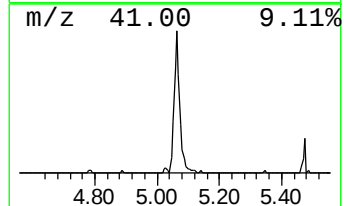
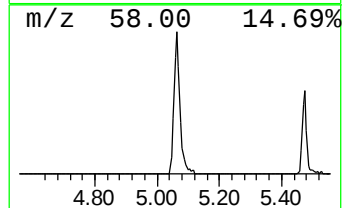
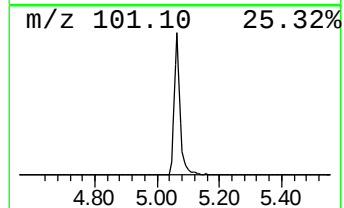
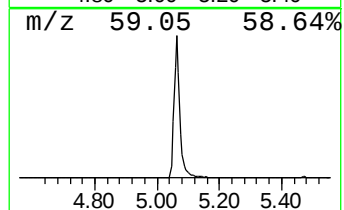
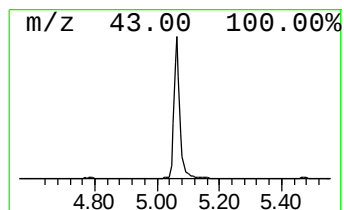
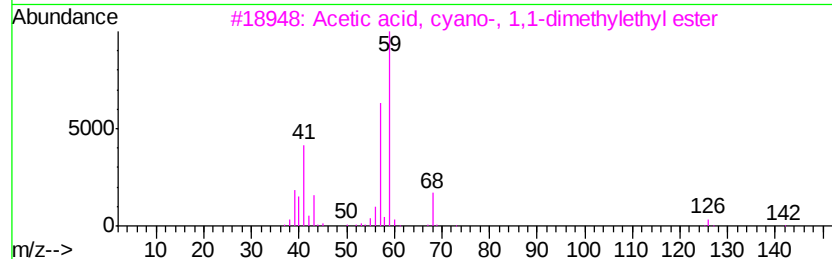
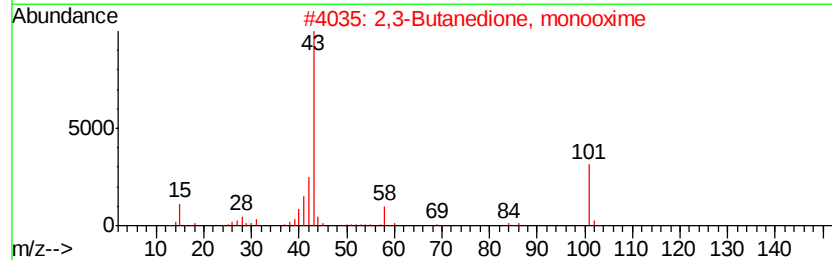
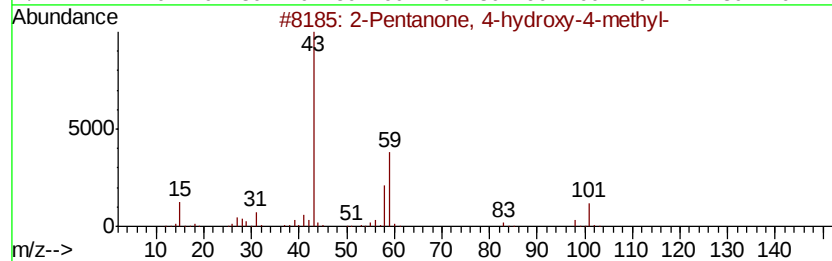
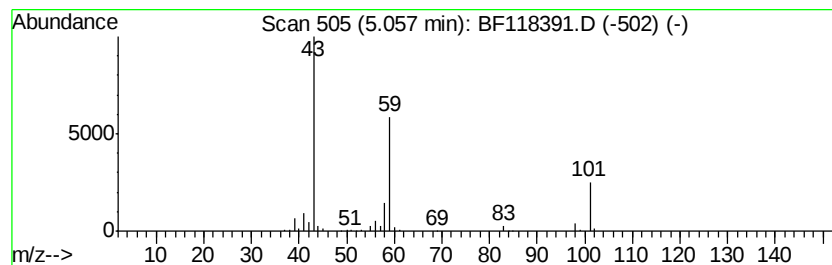
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	14.63 ng	572031	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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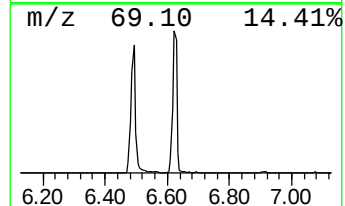
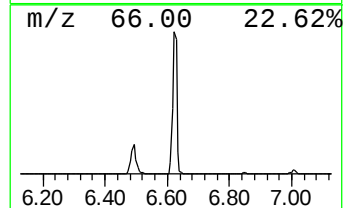
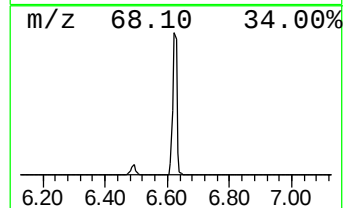
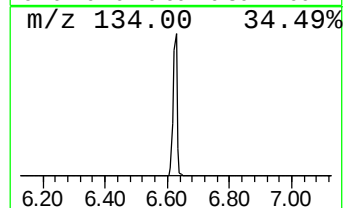
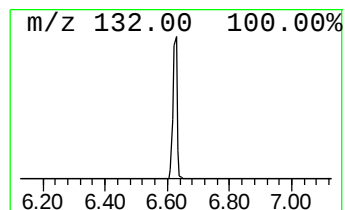
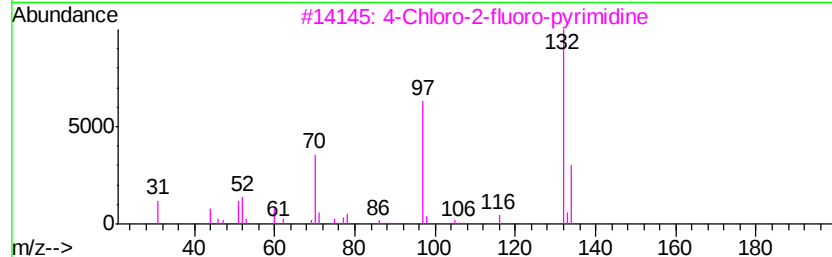
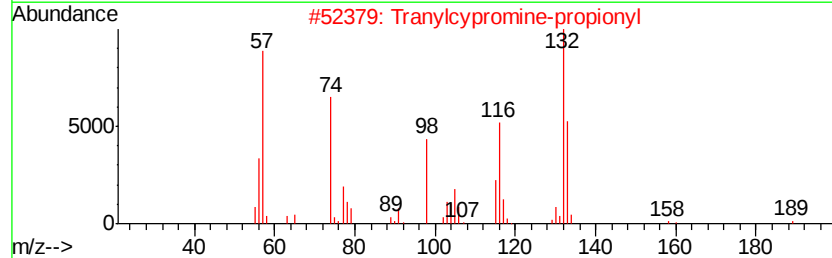
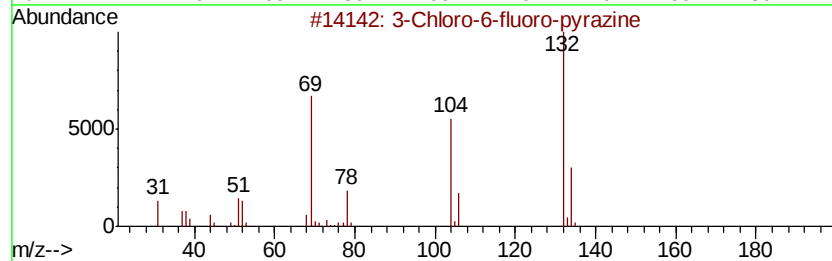
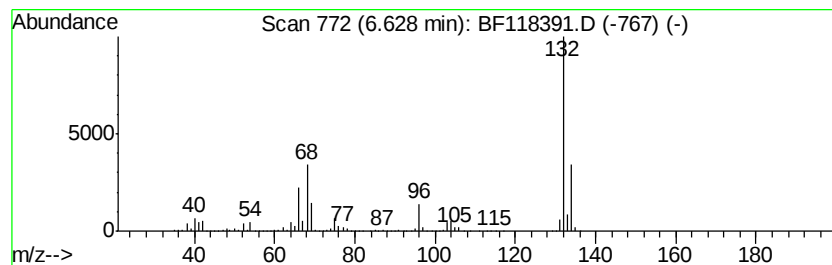
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	82.22 ng	3215270	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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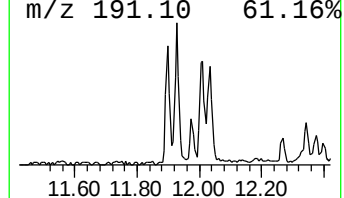
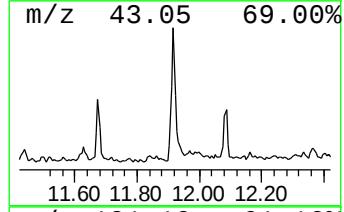
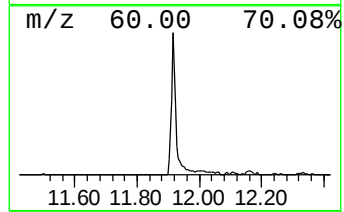
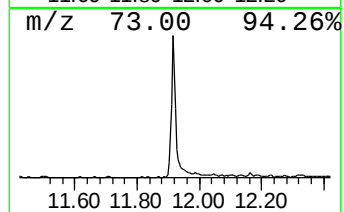
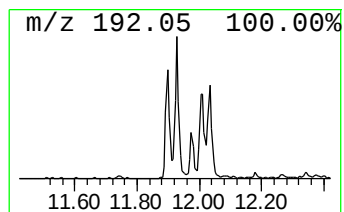
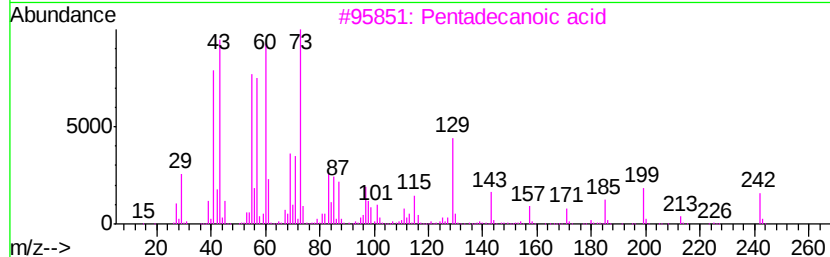
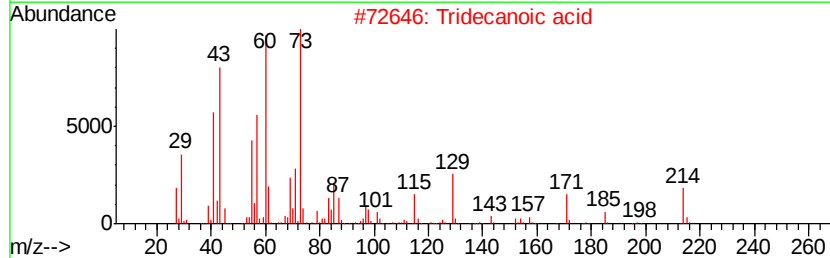
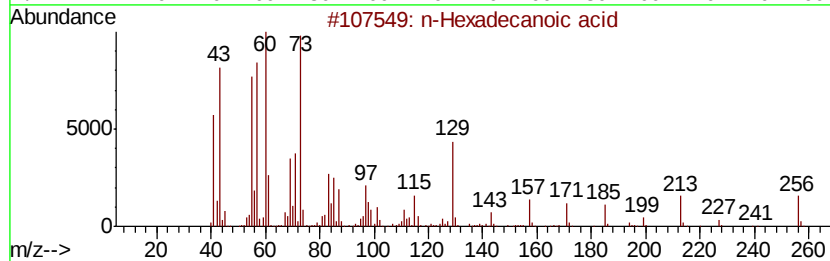
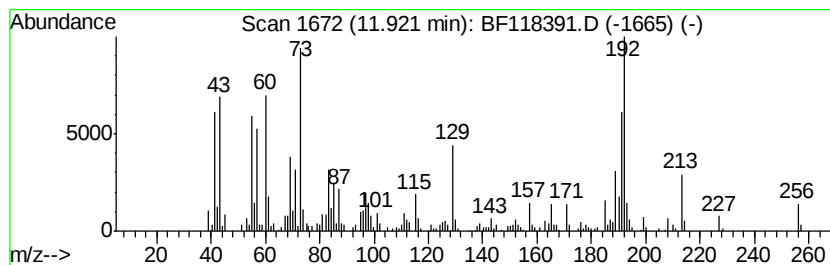
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	9.26 ng	569845	Phenanthrene-d10	11.39	
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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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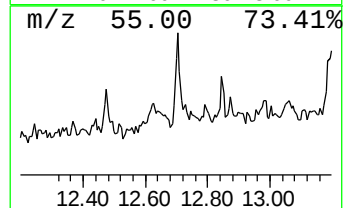
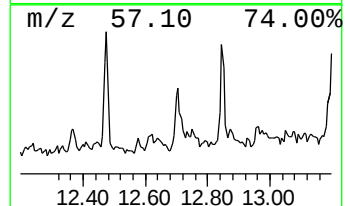
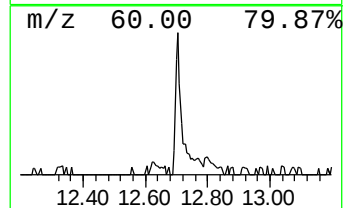
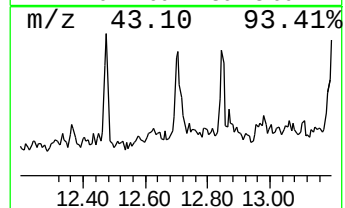
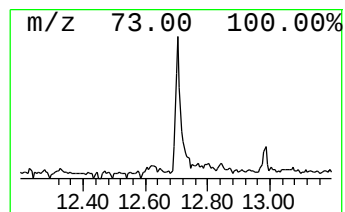
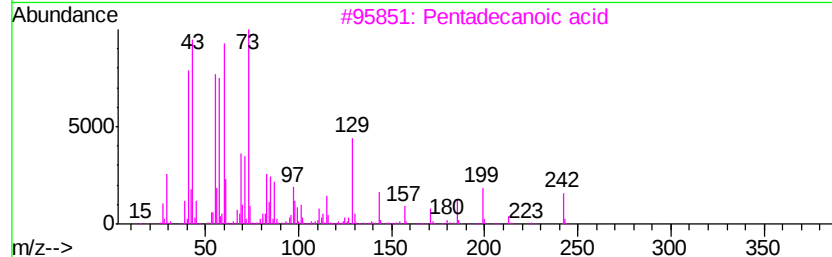
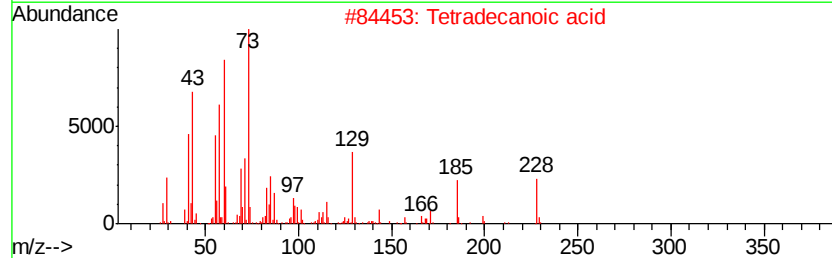
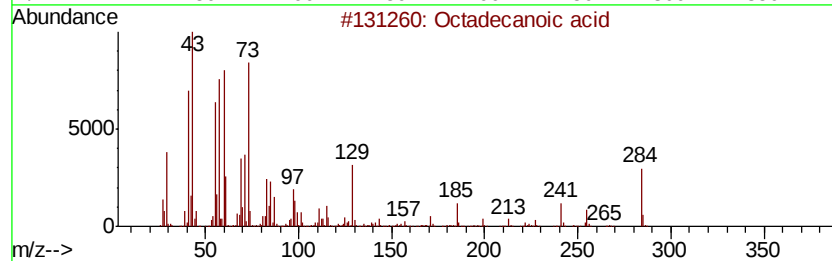
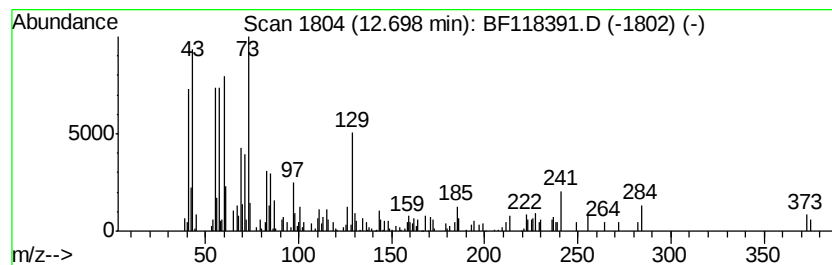
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.37 ng	145659	Phenanthrene-d10	11.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		n-Decanoic acid	172	C10H20O2	000334-48-5	49
5		Tetradecane	198	C14H30	000629-59-4	25



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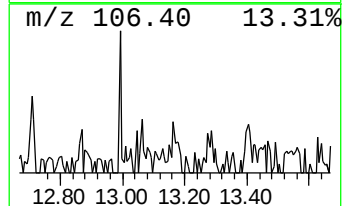
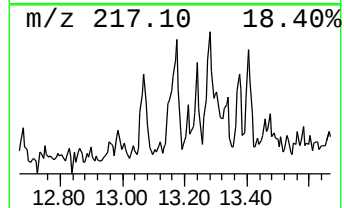
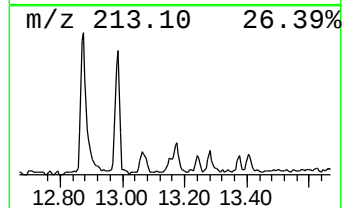
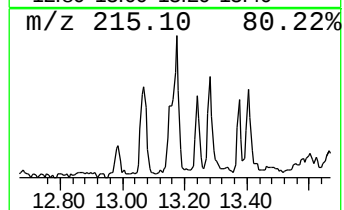
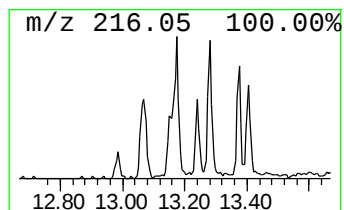
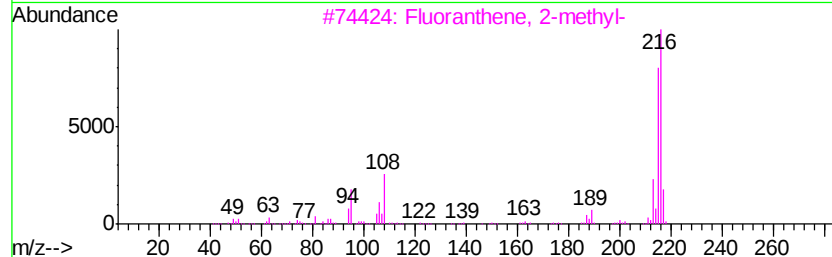
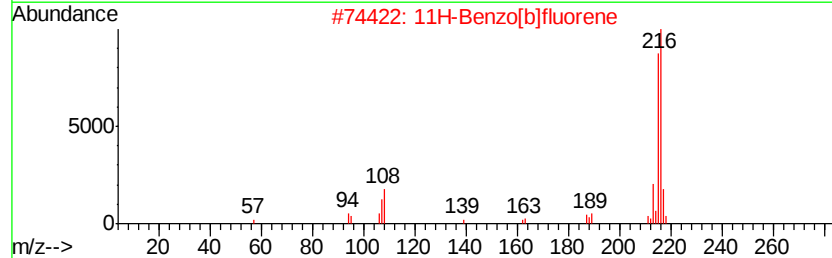
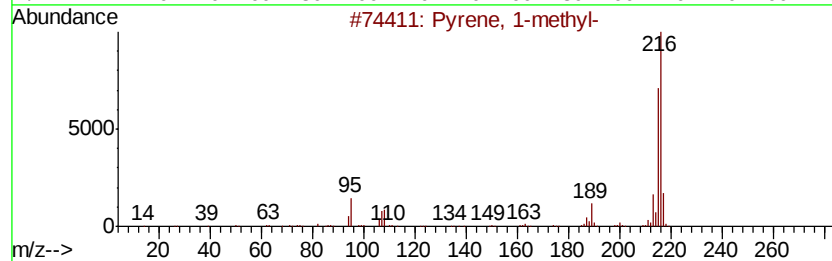
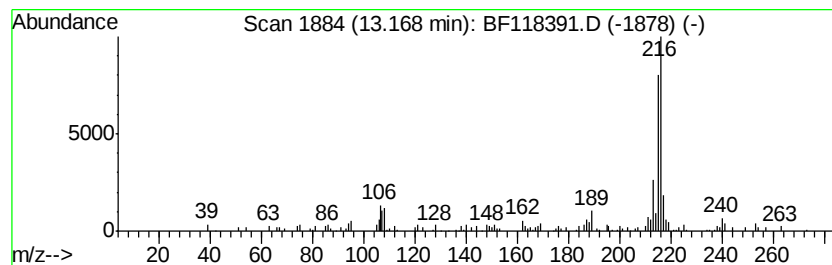
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.17	2.11 ng	118149	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	91
4		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	91
5		Pyrene, 2-methyl-	216	C17H12	003442-78-2	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118391.D
Acq On : 30 Dec 2019 20:01
Operator : JU
Sample : K6455-06
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
K435-WC-1

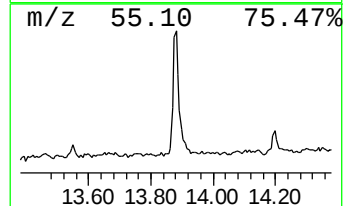
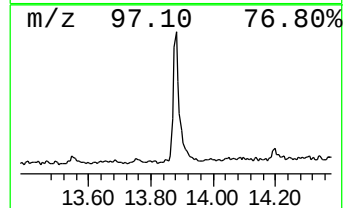
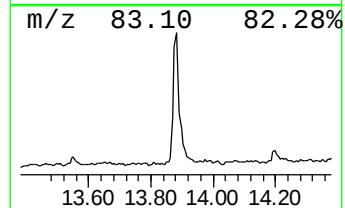
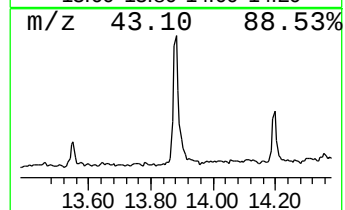
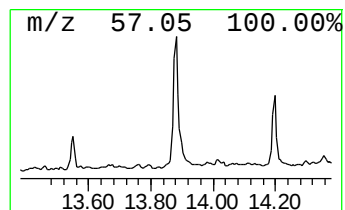
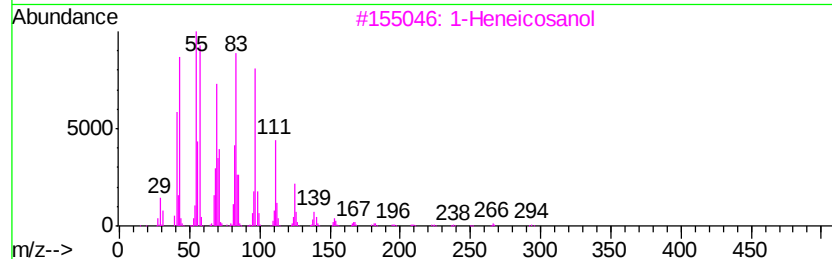
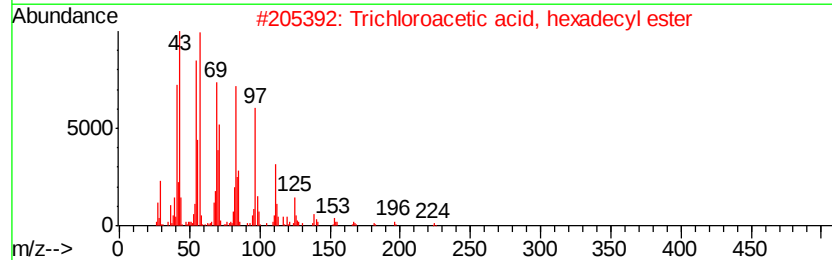
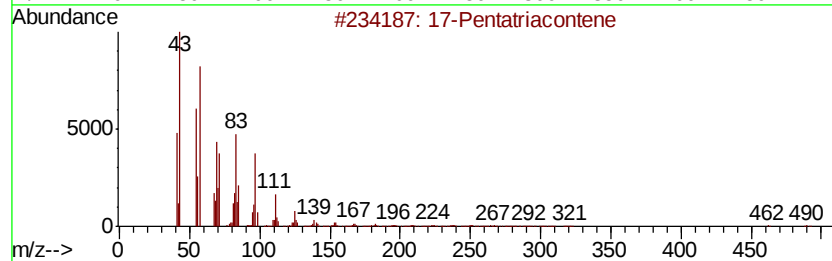
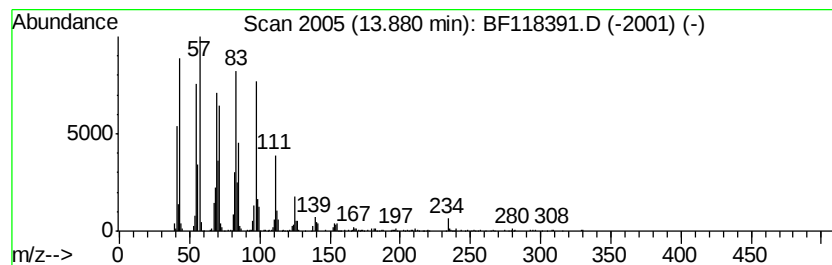
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	16.83 ng	944358	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	17-Pentatriacontene	491	C35H70	006971-40-0	91
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
3		1-Heneicosanol	312	C21H44O	015594-90-8	90
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	81
5		1-Octadecanol	270	C18H38O	000112-92-5	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
 Data File : BF118391.D
 Acq On : 30 Dec 2019 20:01
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 Misc :
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Instrument :
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 ClientSampleId :
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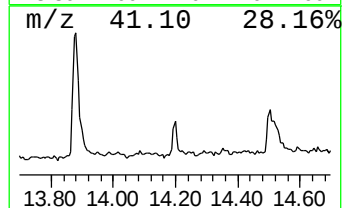
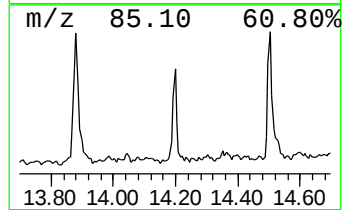
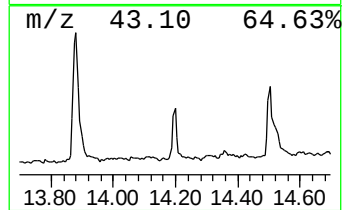
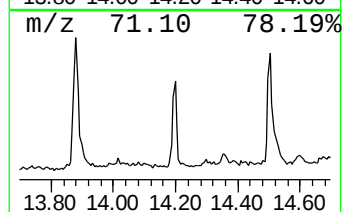
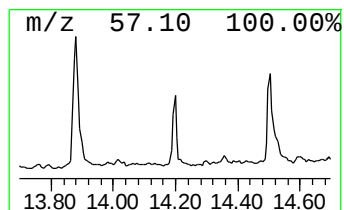
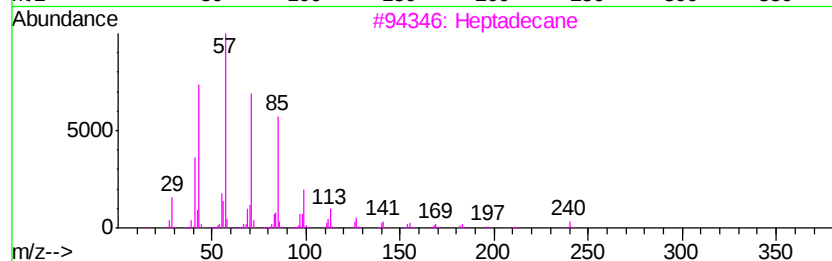
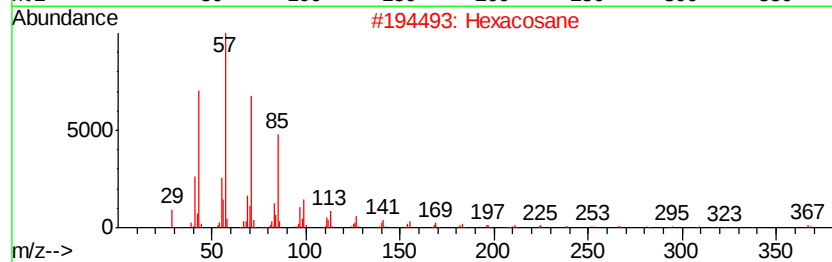
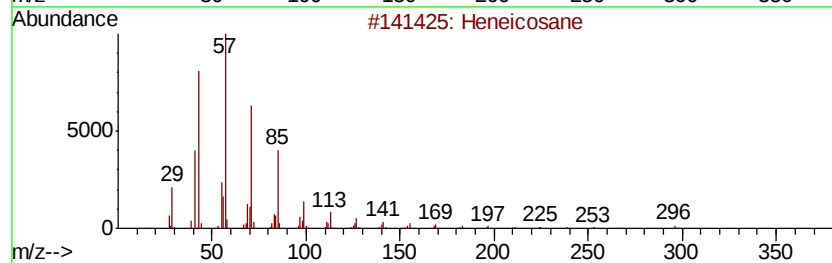
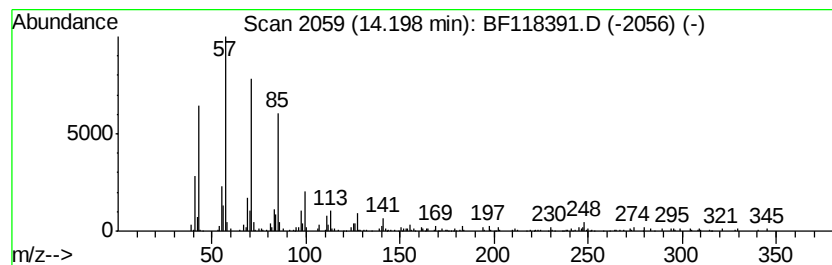
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.74 ng	209705	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	94
2		Hexacosane	366	C26H54	000630-01-3	90
3		Heptadecane	240	C17H36	000629-78-7	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		10-Methylnonadecane	282	C20H42	056862-62-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
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Acq On : 30 Dec 2019 20:01
Operator : JU
Sample : K6455-06
Misc :
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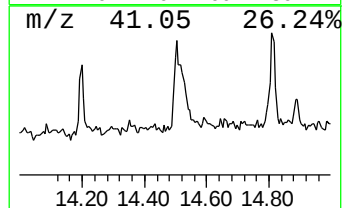
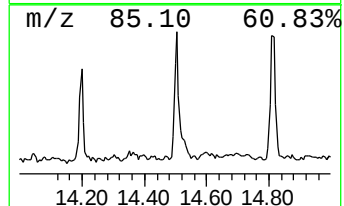
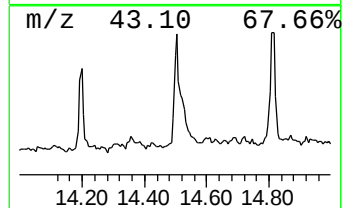
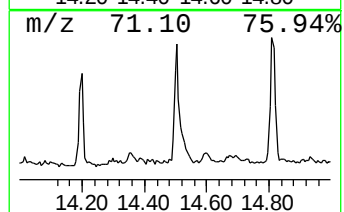
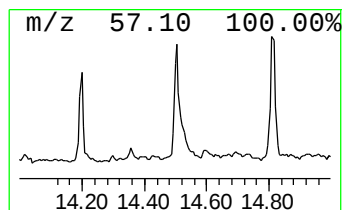
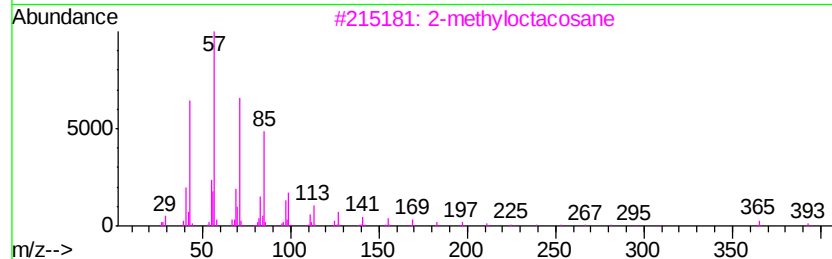
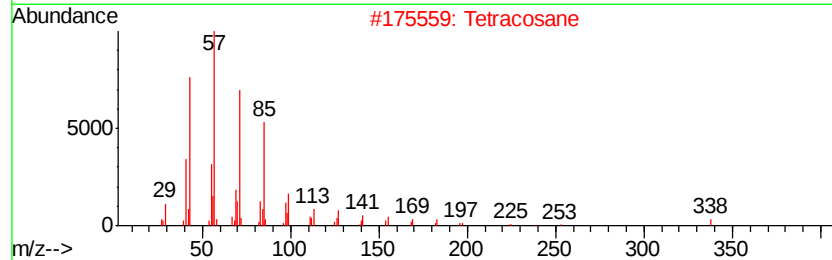
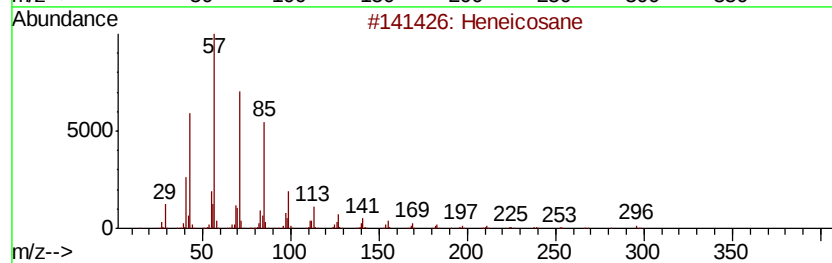
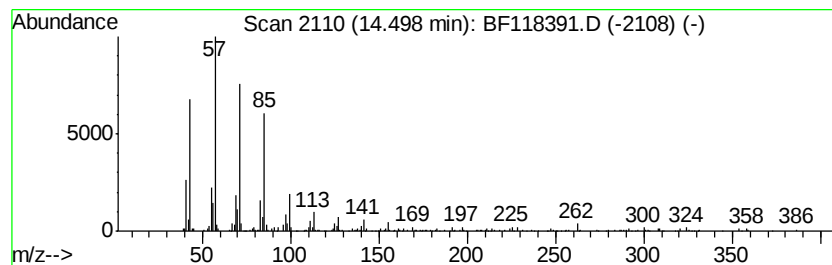
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.50	8.44 ng	473838	Chrysene-d12		14.05
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118391.D
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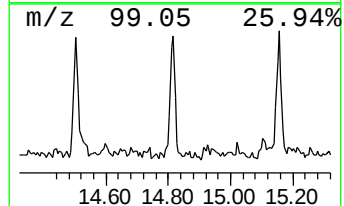
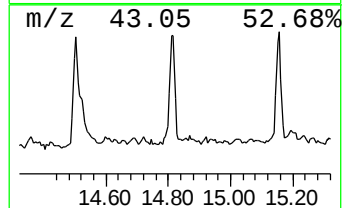
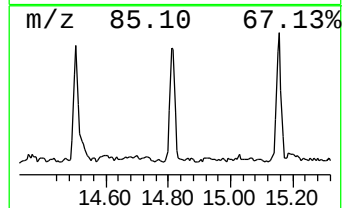
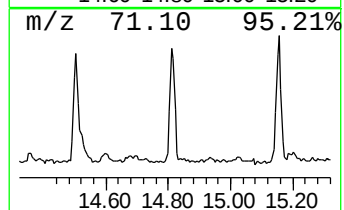
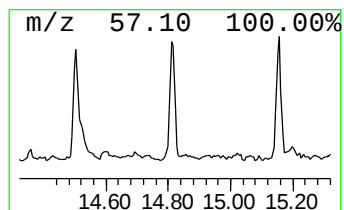
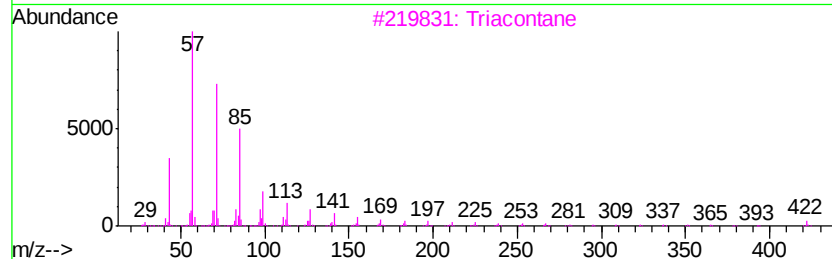
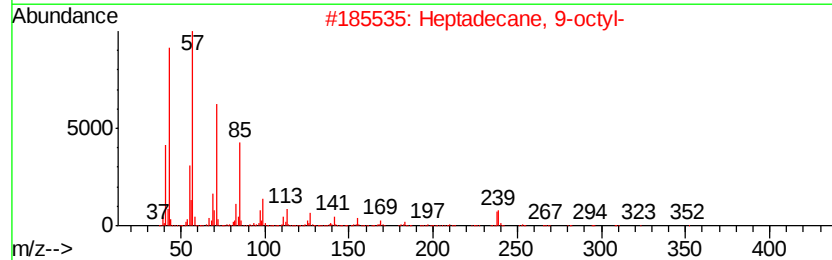
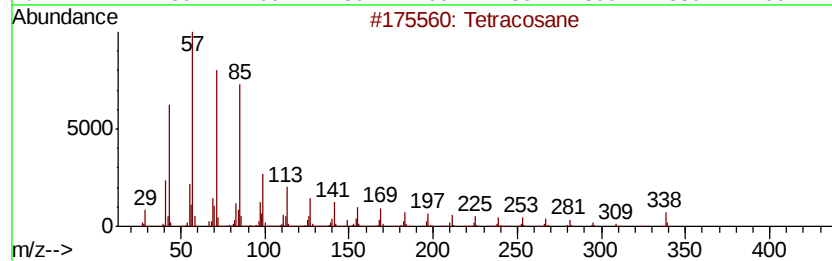
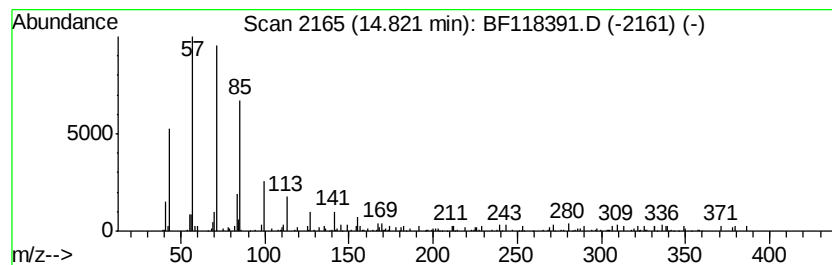
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	3.80 ng	239398	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	94
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Triacontane	422	C30H62	000638-68-6	91
4		Docosane	310	C22H46	000629-97-0	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
Data File : BF118391.D
Acq On : 30 Dec 2019 20:01
Operator : JU
Sample : K6455-06
Misc :
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Instrument :
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ClientSampleId :
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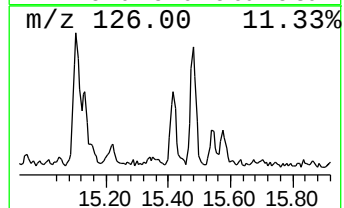
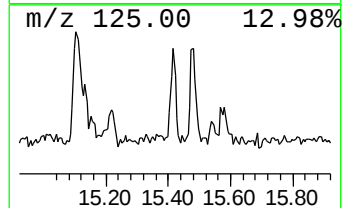
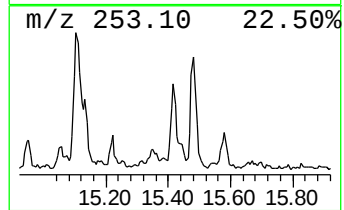
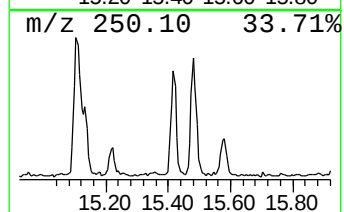
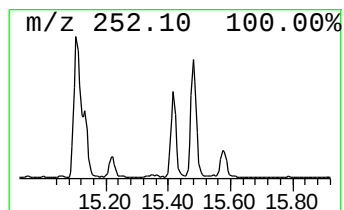
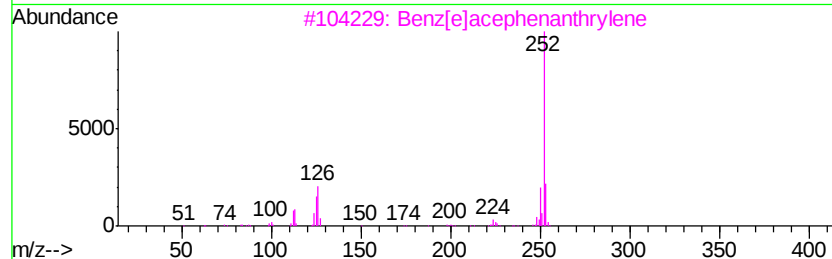
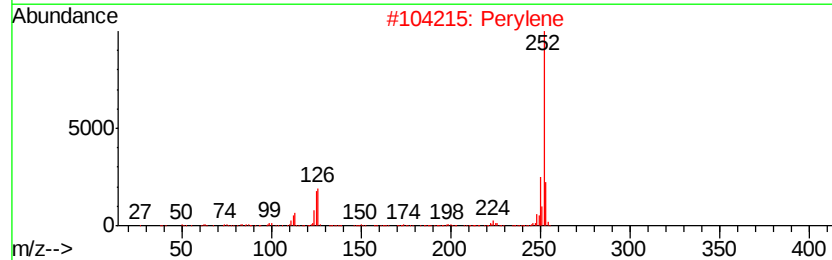
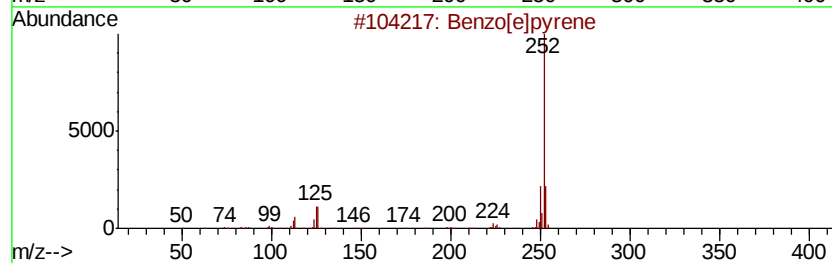
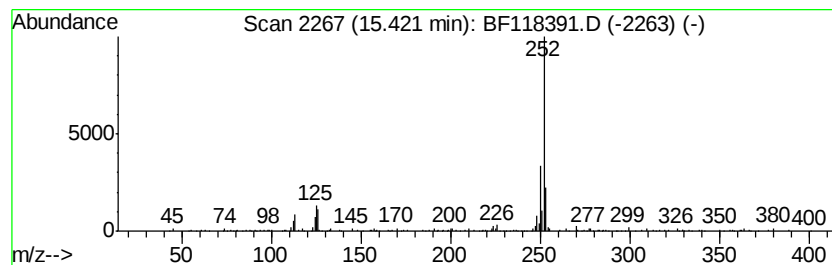
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	2.64 ng	166332	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2		Perylene	252	C20H12	000198-55-0	90
3		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	81
4		Benzo[a]pyrene	252	C20H12	000050-32-8	81
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF123019\
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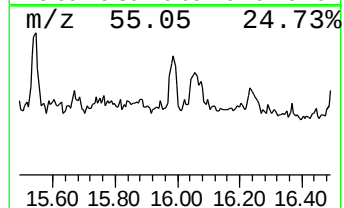
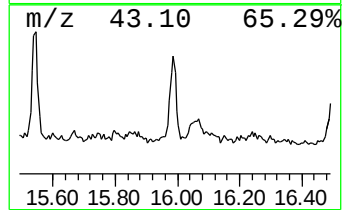
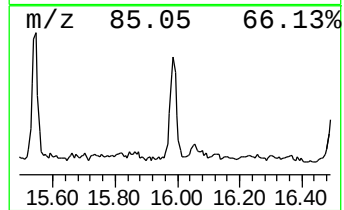
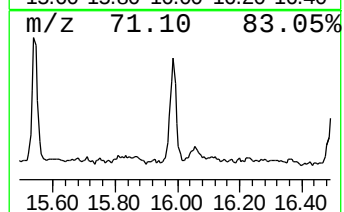
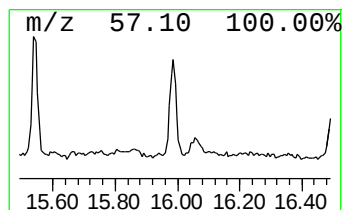
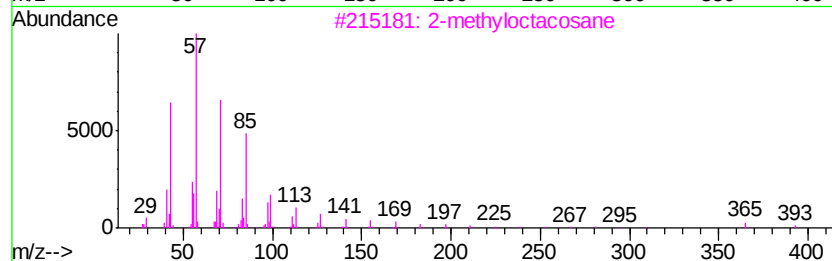
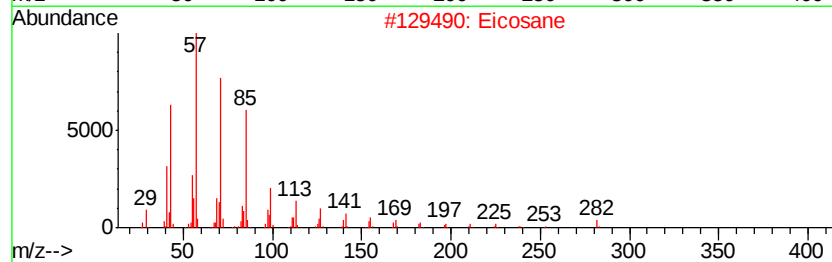
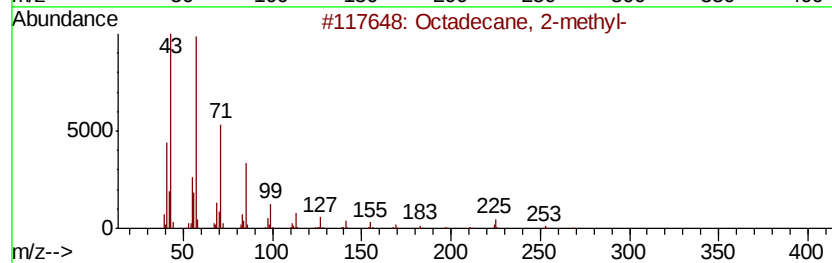
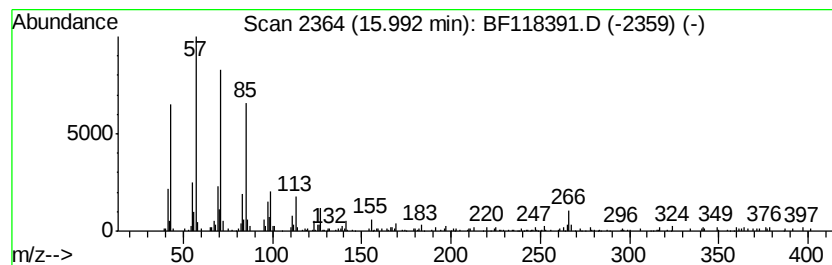
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.99	4.28 ng	269948	Perylene-d12	15.54	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2	Eicosane	282	C20H42	000112-95-8	93
3	2-methyloctacosane	408	C29H60	1000376-72-8	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Hentriacontane	437	C31H64	000630-04-6	87



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ALS Vial : 12 Sample Multiplier: 1

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ClientSampleId :
K435-WC-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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
2-Pentanone, 4-hy...	5.06	14.6	ng	572031	1	6.85	782102	20.0
unknown6.63	6.63	82.2	ng	3215270	1	6.85	782102	20.0
n-Hexadecanoic acid	11.92	9.3	ng	569845	4	11.39	1230280	20.0
Octadecanoic acid	12.70	2.4	ng	145659	4	11.39	1230280	20.0
Pyrene, 1-methyl-	13.17	2.1	ng	118149	5	14.05	1122280	20.0
17-Pentatriacontene	13.88	16.8	ng	944358	5	14.05	1122280	20.0
Heptadecane, 9-oc...	14.20	3.7	ng	209705	5	14.05	1122280	20.0
Hexacosane	14.50	8.4	ng	473838	5	14.05	1122280	20.0
Tetracosane	14.82	3.8	ng	239398	6	15.54	1261510	20.0
Benzo[e]pyrene	15.42	2.6	ng	166332	6	15.54	1261510	20.0
Octadecane, 2-met...	15.99	4.3	ng	269948	6	15.54	1261510	20.0