

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
 Data File : BF117618.D
 Acq On : 30 Oct 2019 12:26
 Operator : JU
 Sample : K5540-09
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 157-14-(0-1.6)

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	5.351	552	555	580	rBV	383256	613405	84.06%	7.913%
2	6.381	727	730	747	rBV	480224	683078	93.61%	8.812%
3	6.504	747	751	758	rVB	755005	729724	100.00%	9.414%
4	6.728	785	789	798	rBV	196933	192759	26.42%	2.487%
5	6.881	812	815	829	rBV	578943	517198	70.88%	6.672%
6	7.292	882	885	912	rBV	336053	452201	61.97%	5.834%
7	8.010	1004	1007	1033	rBV	191255	250574	34.34%	3.232%
8	9.080	1185	1189	1202	rBV	625112	592474	81.19%	7.643%
9	9.480	1254	1257	1266	rBV	61943	62661	8.59%	0.808%
10	9.757	1301	1304	1318	rBV	270846	279160	38.26%	3.601%
11	10.557	1436	1440	1452	rBV	313991	366564	50.23%	4.729%
12	11.245	1554	1557	1560	rBV	216868	232313	31.84%	2.997%
13	11.274	1560	1562	1568	rVV	105406	103162	14.14%	1.331%
14	11.327	1568	1571	1576	rVB2	13381	15871	2.17%	0.205%
15	11.498	1595	1600	1604	rBV2	5267	8455	1.16%	0.109%
16	11.751	1641	1643	1645	rBV	15774	14616	2.00%	0.189%
17	11.774	1645	1647	1654	rVB2	66254	77810	10.66%	1.004%
18	11.863	1659	1662	1665	rVV2	23366	29624	4.06%	0.382%
19	11.886	1665	1666	1672	rVB	13404	11266	1.54%	0.145%
20	12.304	1734	1737	1739	rBV	10730	11827	1.62%	0.153%
21	12.404	1749	1754	1756	rBV4	6895	9467	1.30%	0.122%
22	12.463	1761	1764	1770	rBV	159082	157102	21.53%	2.027%
23	12.557	1778	1780	1784	rBV4	15933	19204	2.63%	0.248%
24	12.616	1788	1790	1794	rVV5	11041	15339	2.10%	0.198%
25	12.692	1798	1803	1809	rVV	155100	172541	23.64%	2.226%
26	12.751	1809	1813	1815	rVB5	6713	8595	1.18%	0.111%
27	12.827	1822	1826	1831	rBV	456616	407911	55.90%	5.262%
28	12.916	1837	1841	1846	rVB3	10907	16599	2.27%	0.214%
29	12.998	1851	1855	1856	rBV3	8488	8382	1.15%	0.108%
30	13.021	1857	1859	1862	rVB	12526	10827	1.48%	0.140%
31	13.127	1873	1877	1881	rBV4	15032	21409	2.93%	0.276%
32	13.221	1890	1893	1896	rBV3	11202	10562	1.45%	0.136%
33	13.257	1896	1899	1902	rBV4	10353	15439	2.12%	0.199%
34	13.292	1904	1905	1909	rVB3	7717	8330	1.14%	0.107%

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35	13.545	1943	1948	1954	rVB	12720	16389	2.25%	0.211%
36	13.651	1963	1966	1967	rBV2	10418	10756	1.47%	0.139%
37	13.663	1967	1968	1971	rVV2	14928	10808	1.48%	0.139%
38	13.739	1975	1981	1990	rVB7	47016	110221	15.10%	1.422%
39	13.857	1998	2001	2003	rBV	18173	19414	2.66%	0.250%
40	13.892	2003	2007	2010	rVV2	269011	330043	45.23%	4.258%
41	13.915	2010	2011	2018	rVB	73520	73693	10.10%	0.951%
42	13.998	2023	2025	2029	rVB2	9944	11010	1.51%	0.142%
43	14.039	2029	2032	2034	rBV2	16195	16757	2.30%	0.216%
44	14.063	2034	2036	2041	rVV6	9376	12003	1.64%	0.155%
45	14.286	2072	2074	2077	rVB2	14933	12379	1.70%	0.160%
46	14.345	2081	2084	2088	rVV3	32965	42394	5.81%	0.547%
47	14.639	2128	2134	2137	rBV2	51979	65042	8.91%	0.839%
48	14.710	2143	2146	2148	rBV2	15408	14808	2.03%	0.191%
49	14.921	2179	2182	2185	rBV	65979	94108	12.90%	1.214%
50	14.951	2185	2187	2195	rVB2	94007	116333	15.94%	1.501%
51	15.027	2198	2200	2206	rVB3	15784	19187	2.63%	0.248%
52	15.210	2228	2231	2235	rBV	31733	39195	5.37%	0.506%
53	15.274	2239	2242	2245	rVV	48589	62919	8.62%	0.812%
54	15.333	2245	2252	2264	rVB2	180014	352303	48.28%	4.545%
55	15.498	2278	2280	2283	rBV3	10905	11216	1.54%	0.145%
56	15.709	2313	2316	2321	rVB	39842	53796	7.37%	0.694%
57	16.180	2392	2396	2400	rBV4	19306	30385	4.16%	0.392%
58	16.345	2420	2424	2429	rVB7	16386	27308	3.74%	0.352%
59	16.751	2486	2493	2500	rVB6	20487	49711	6.81%	0.641%
60	16.892	2512	2517	2522	rVB9	10895	23086	3.16%	0.298%

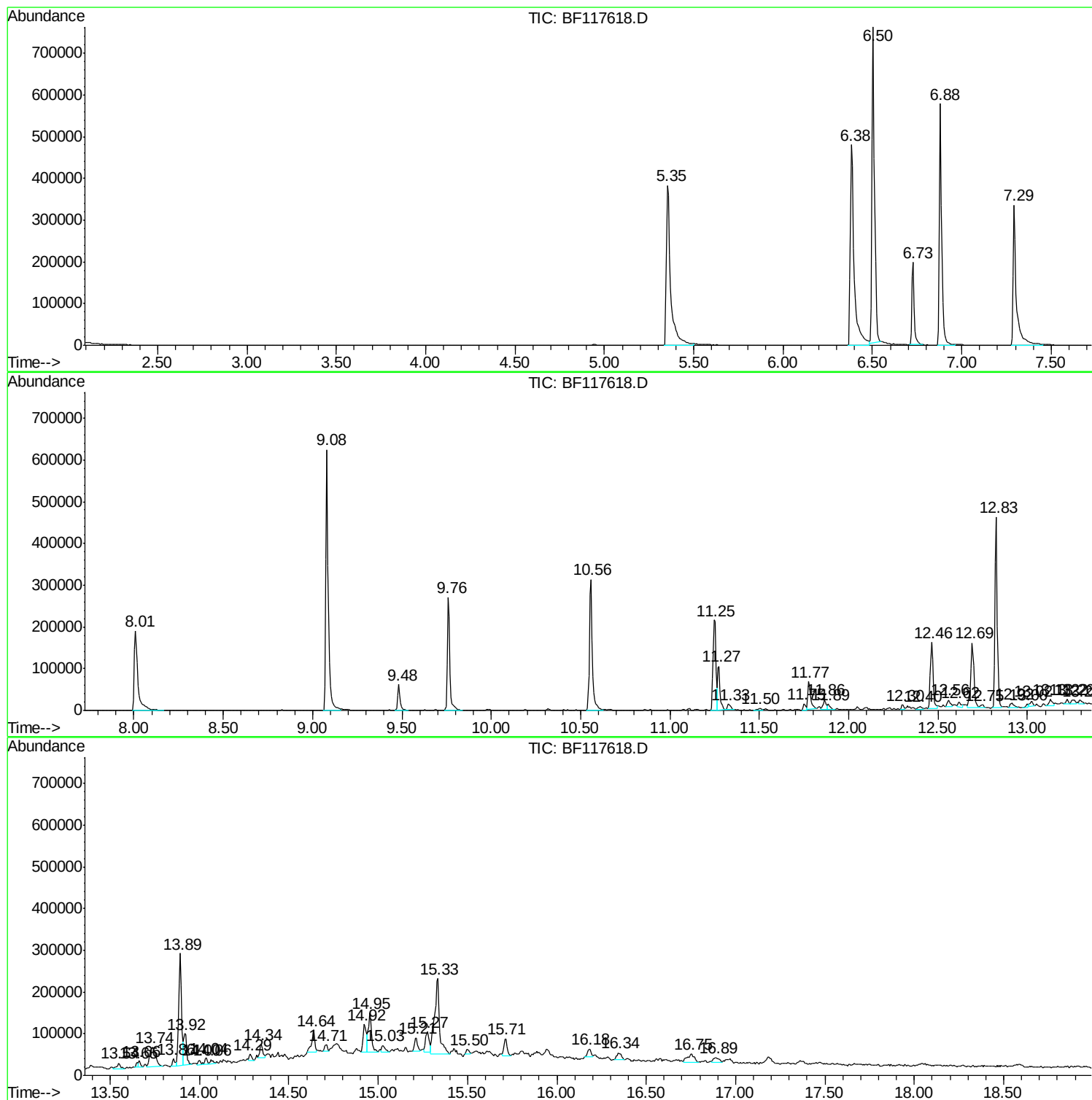
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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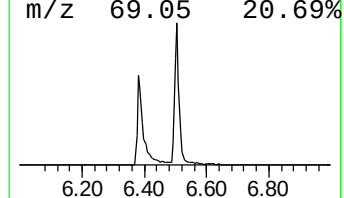
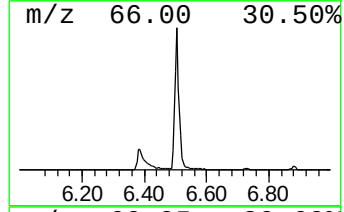
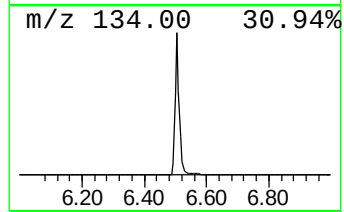
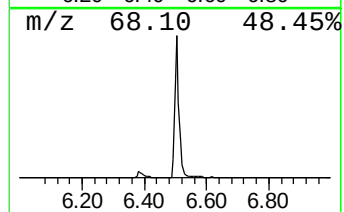
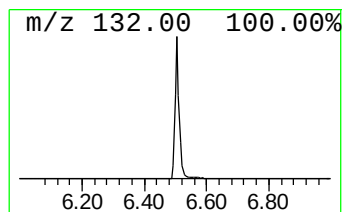
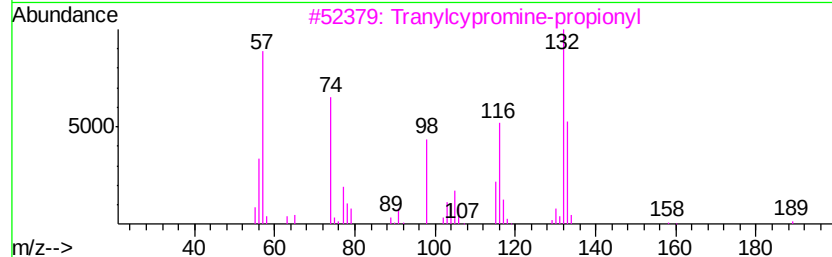
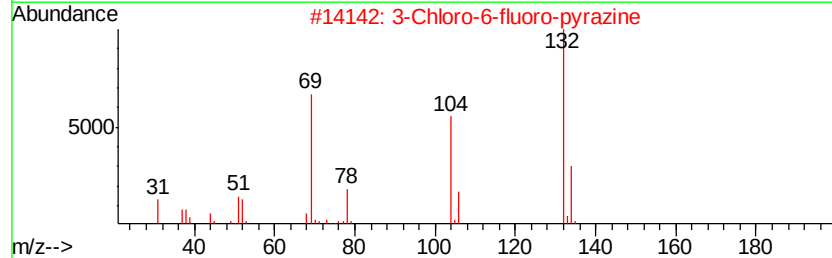
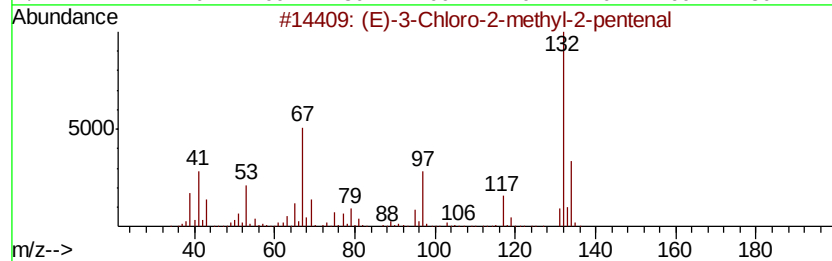
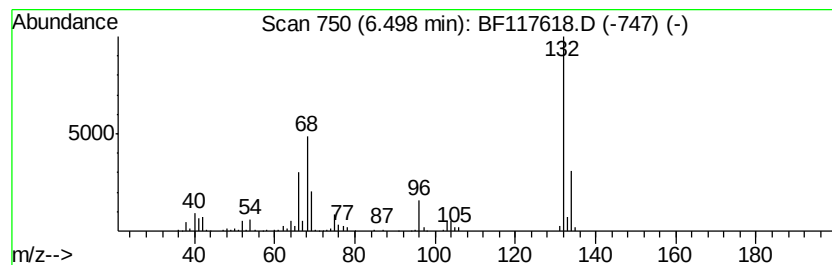
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	75.71 ng	729724	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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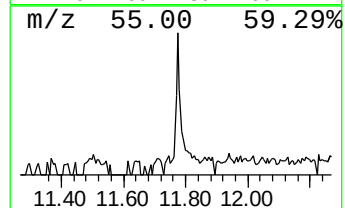
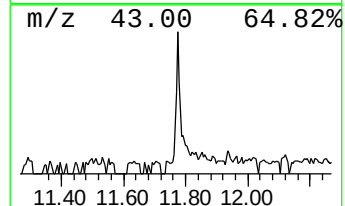
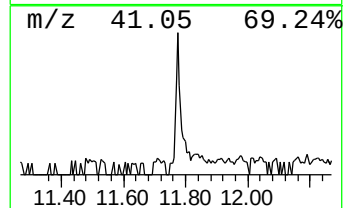
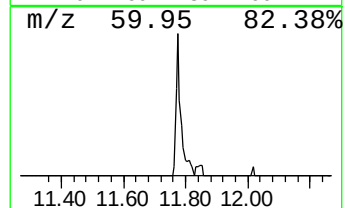
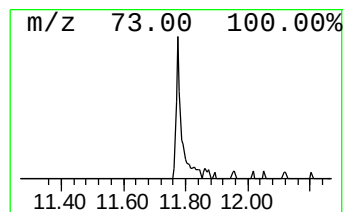
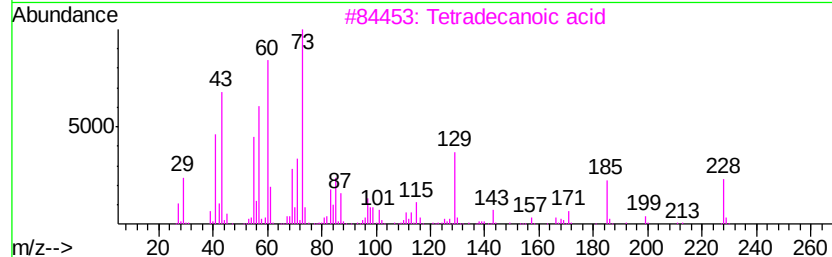
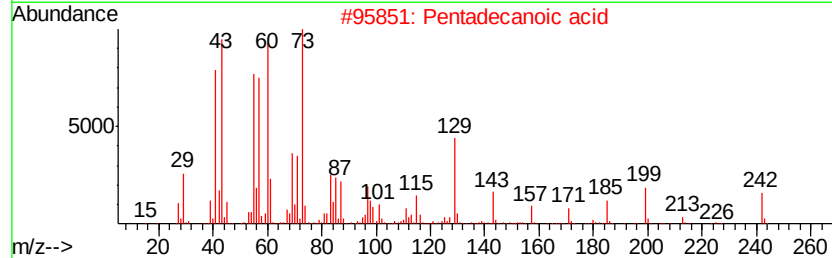
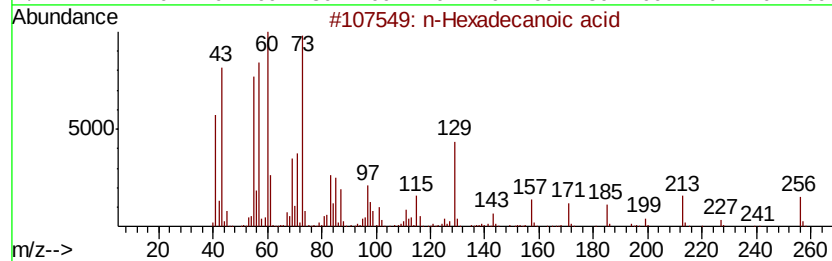
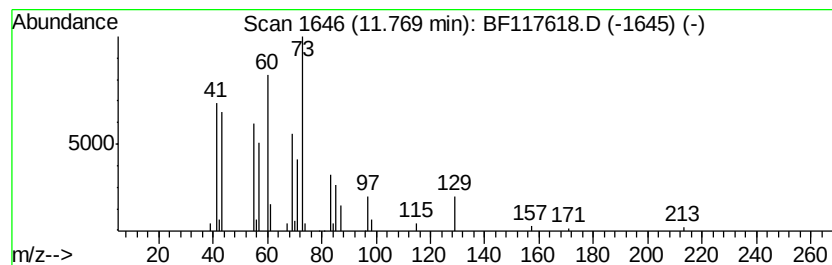
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.77	6.70 ng	77810	Phenanthrene-d10	11.25	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58



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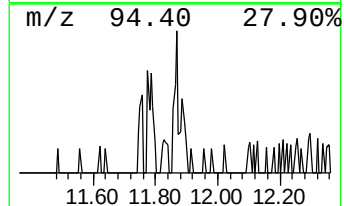
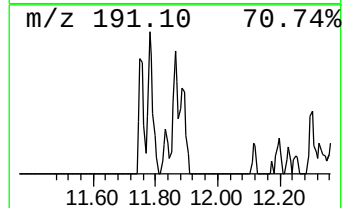
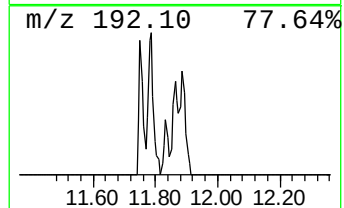
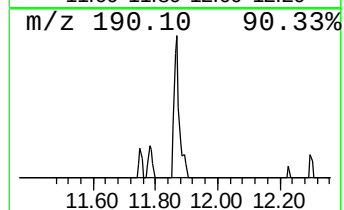
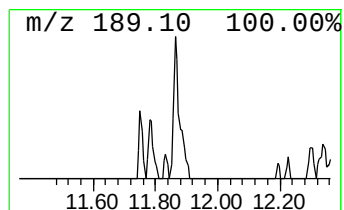
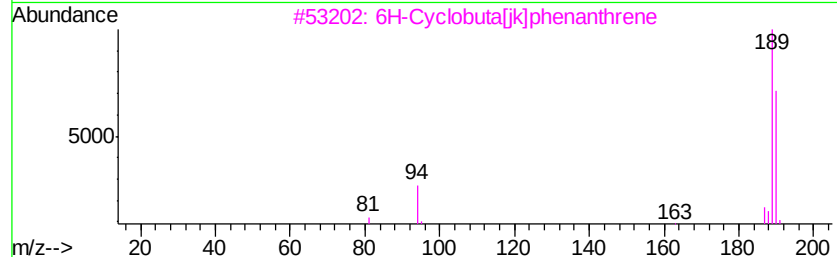
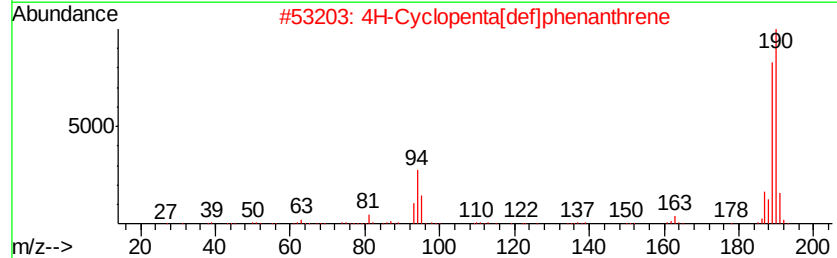
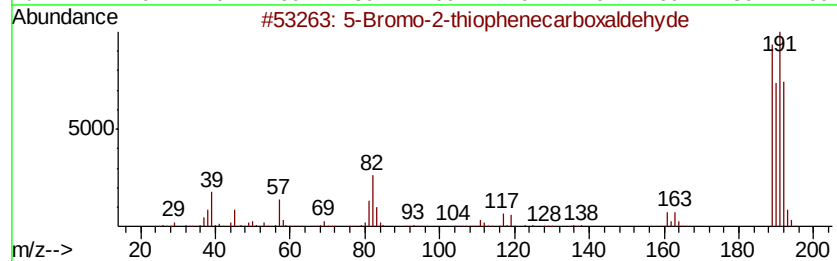
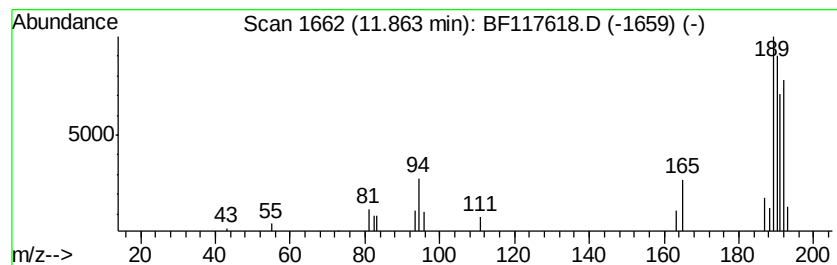
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 5-Bromo-2-thiophenecarboxal... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.		
11.86	2.55 ng	29624	Phenanthrene-d10		11.25		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	58		
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49		
3	6H-Cyclobuta[f]phenanthrene	190	C15H10	083469-43-6	49		
4	Benzene, 1,1'-(1,2-propadienylid...	192	C15H12	014251-57-1	38		
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	38		



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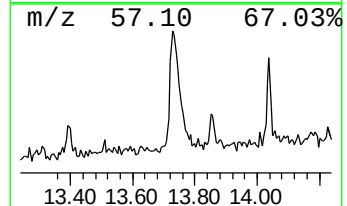
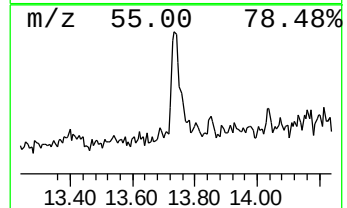
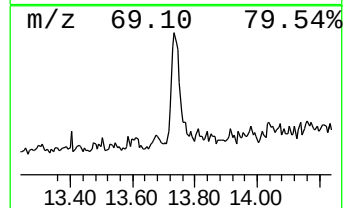
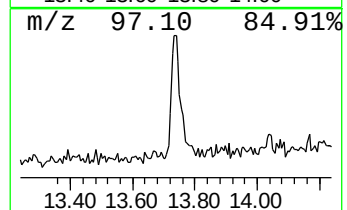
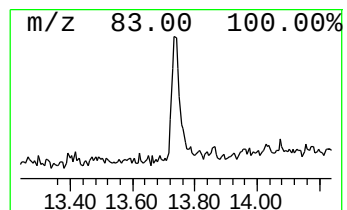
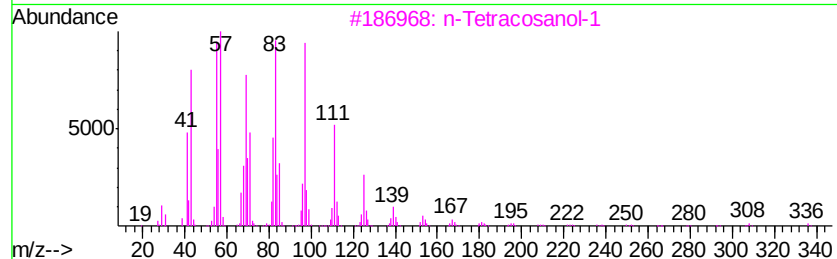
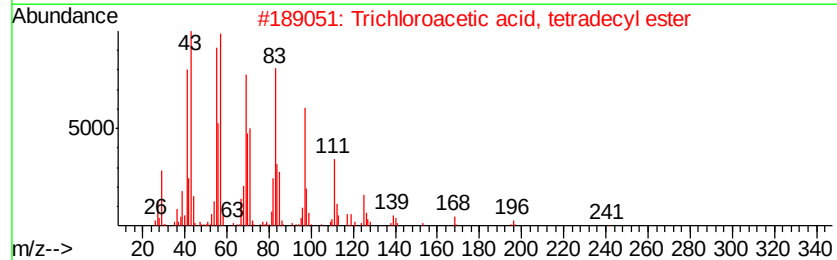
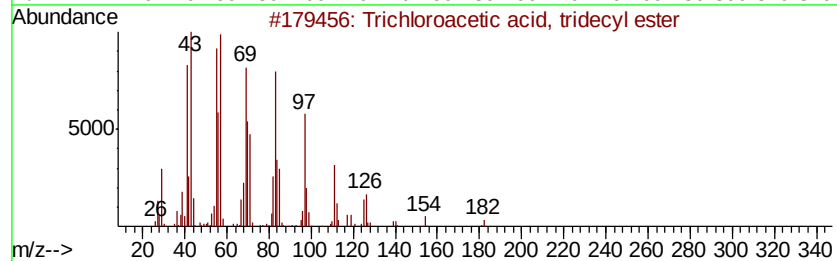
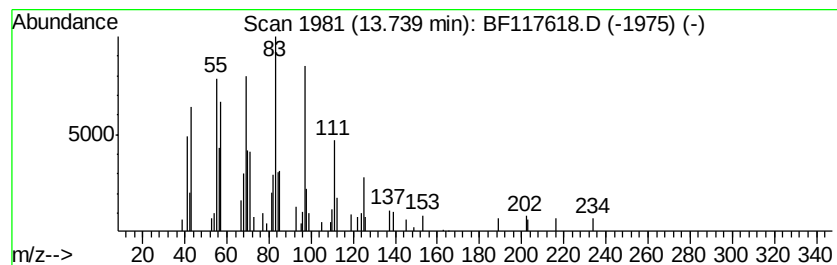
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Trichloroacetic acid, tride... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.74	6.68 ng	110221	Chrysene-d12		13.89	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, tridecyl e...	344	C15H27Cl3O2	074339-51-8	91
2		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	90
4		1-Heptacosanol	396	C27H56O	002004-39-9	87
5		Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87



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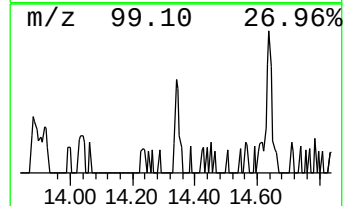
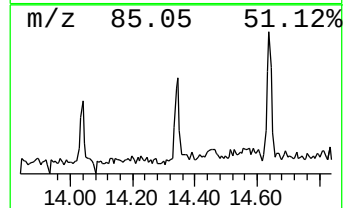
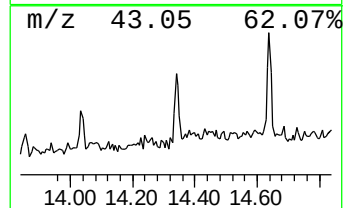
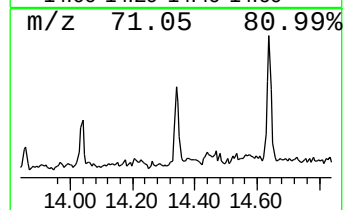
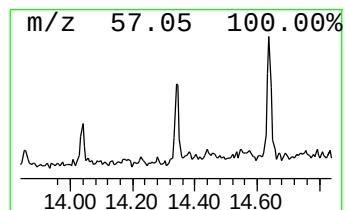
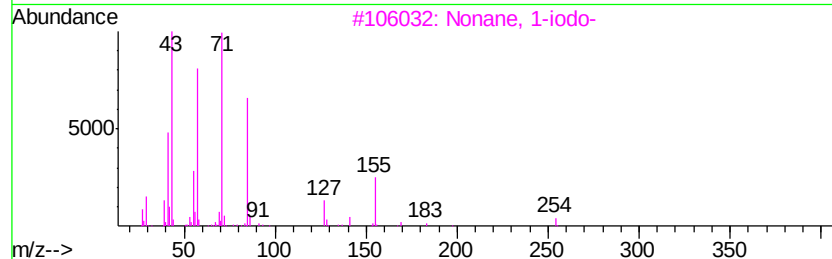
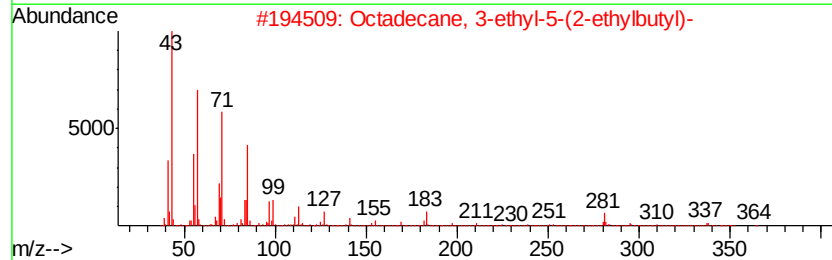
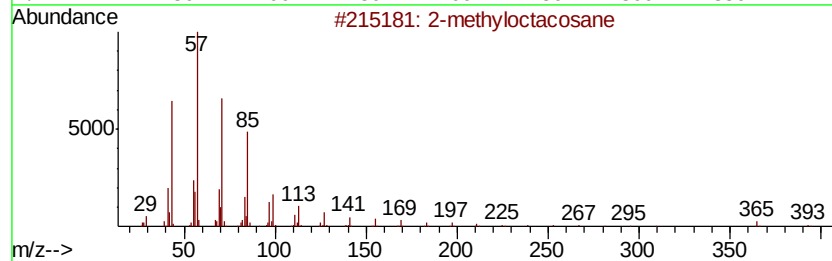
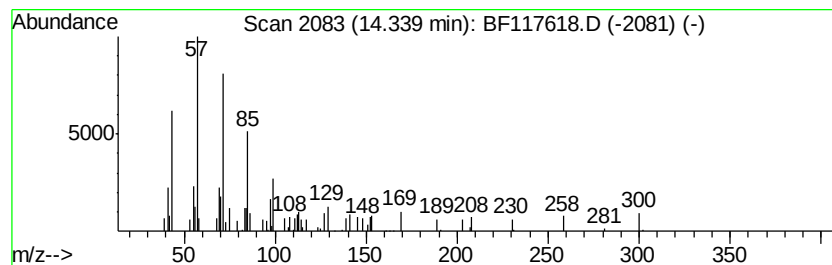
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.57 ng	42394	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	50
2		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	50
3		Nonane, 1-iodo-	254	C9H19I	004282-42-2	38
4		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	38
5		Decane, 2,3,7-trimethyl-	184	C13H28	062238-13-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117618.D
Acq On : 30 Oct 2019 12:26
Operator : JU
Sample : K5540-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
157-14-(0-1.6)

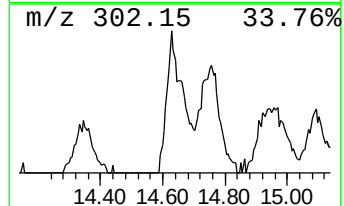
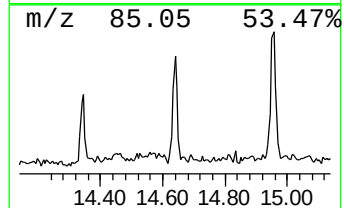
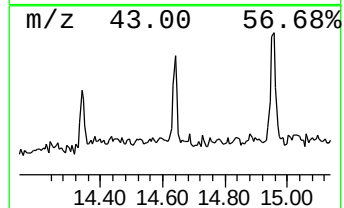
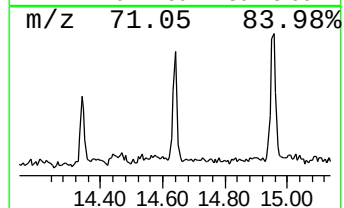
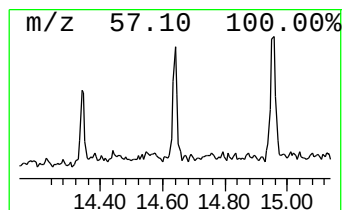
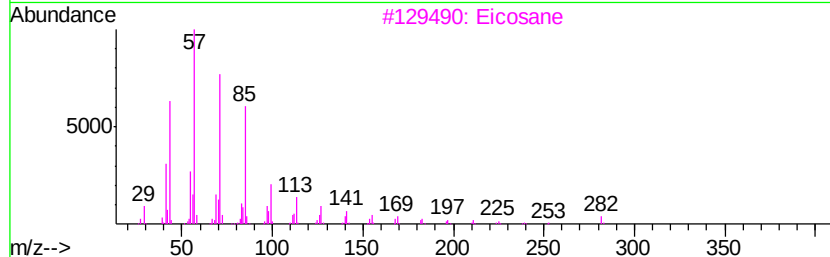
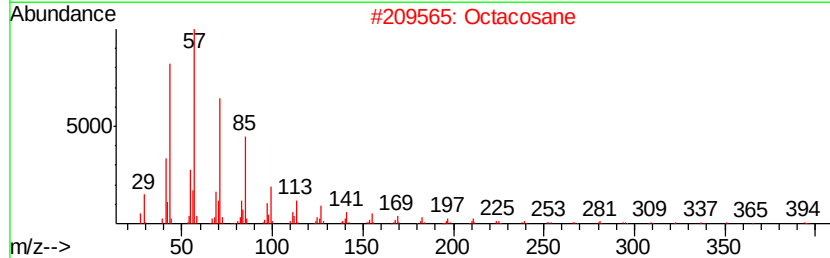
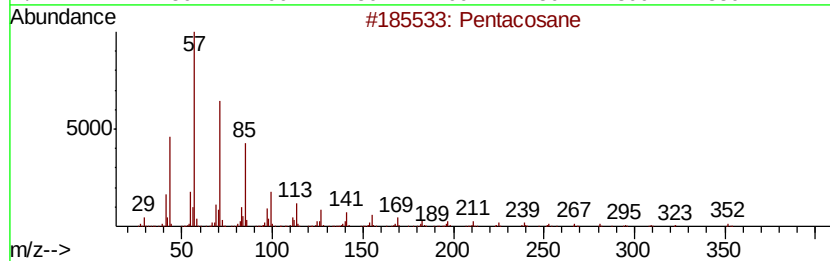
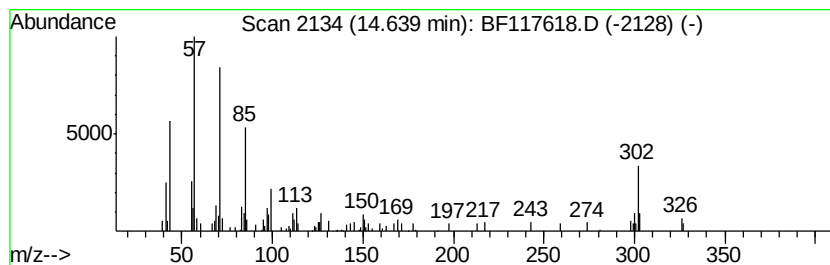
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.69 ng	65042	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane		352	C25H52	000629-99-2	70
2	Octacosane		394	C28H58	000630-02-4	62
3	Eicosane		282	C20H42	000112-95-8	62
4	Heptadecane		240	C17H36	000629-78-7	62
5	Hexadecane		226	C16H34	000544-76-3	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117618.D
Acq On : 30 Oct 2019 12:26
Operator : JU
Sample : K5540-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
157-14-(0-1.6)

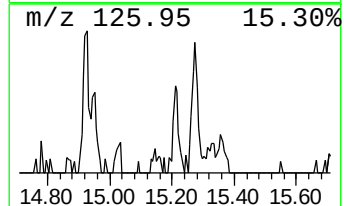
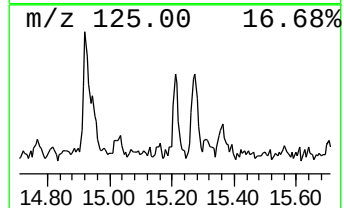
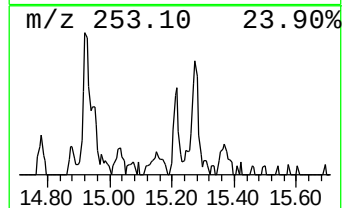
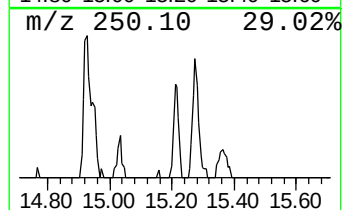
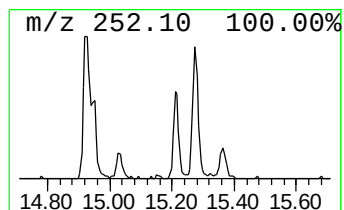
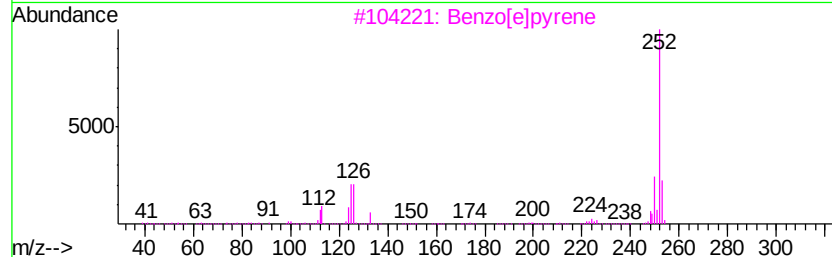
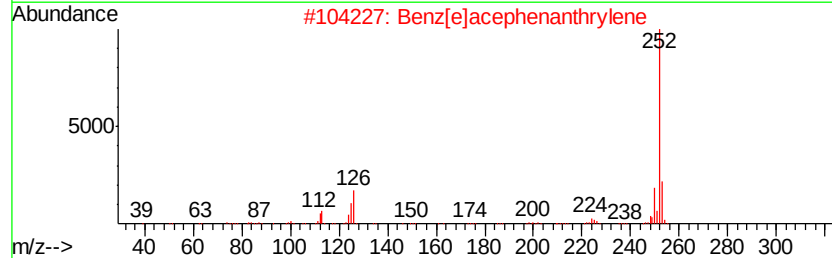
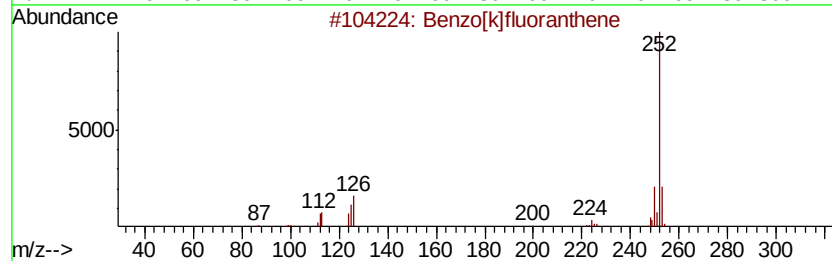
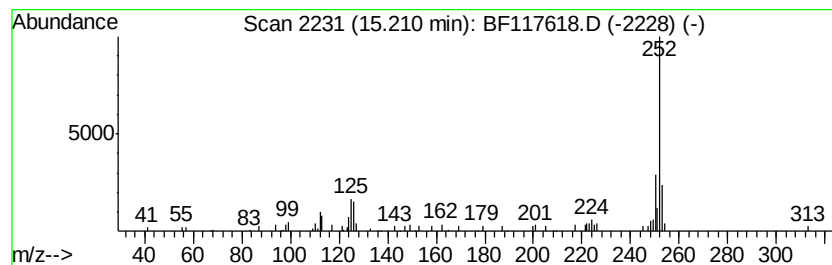
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.21	2.23 ng	39195	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[k]fluoranthene	252	C20H12	000207-08-9	94
2		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
3		Benzo[e]pyrene	252	C20H12	000192-97-2	81
4		Perylene	252	C20H12	000198-55-0	81
5		Benzo[a]pyrene	252	C20H12	000050-32-8	81



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103019\
Data File : BF117618.D
Acq On : 30 Oct 2019 12:26
Operator : JU
Sample : K5540-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
157-14-(0-1.6)

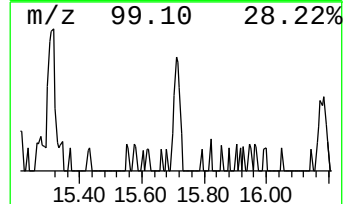
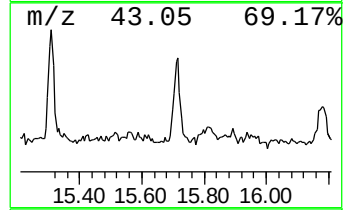
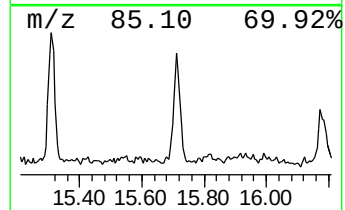
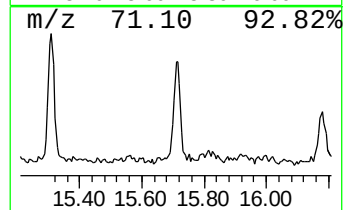
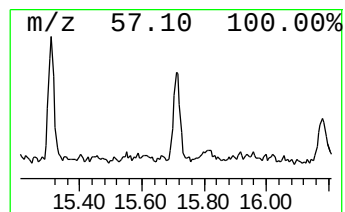
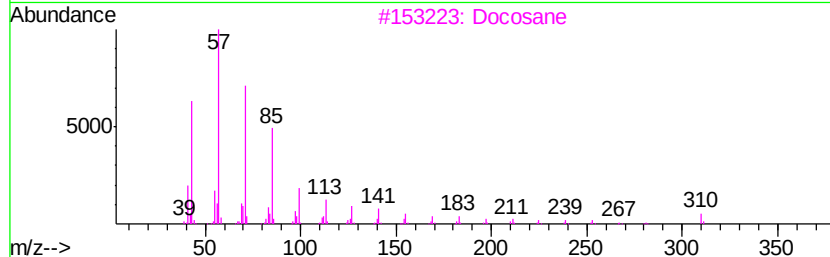
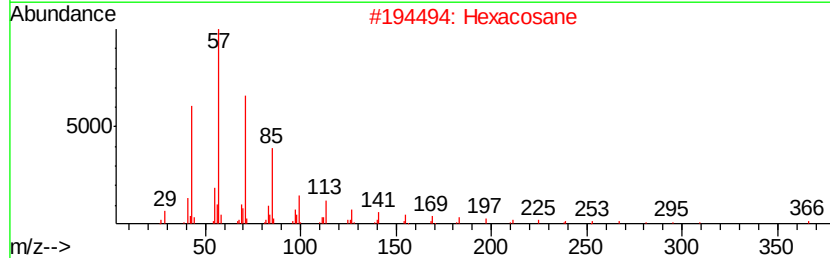
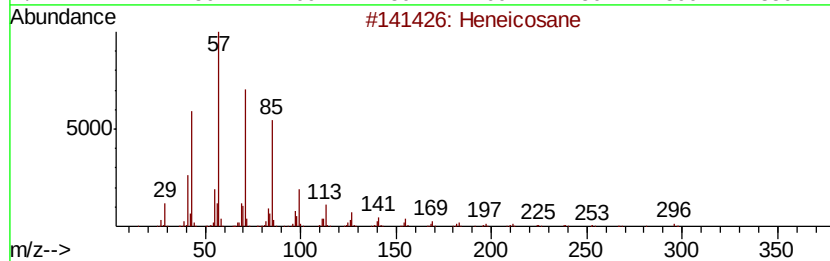
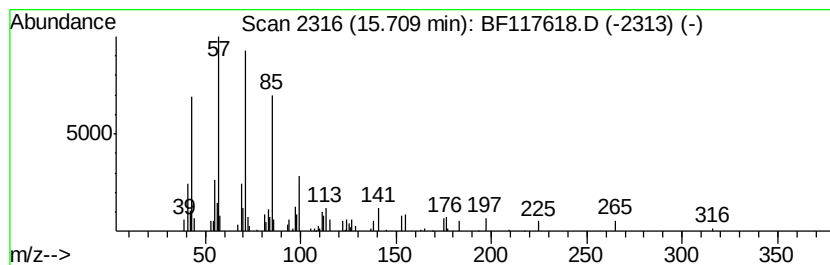
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	3.05 ng	53796	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	86
2	Hexacosane		366	C26H54	000630-01-3	86
3	Docosane		310	C22H46	000629-97-0	80
4	Undecane, 2,9-dimethyl-		184	C13H28	017301-26-7	72
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103019\
Data File : BF117618.D
Acq On : 30 Oct 2019 12:26
Operator : JU
Sample : K5540-09
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
157-14-(0-1.6)

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
unknown6.50	6.50	75.7	ng	729724	1	6.73	192759	20.0
n-Hexadecanoic acid	11.77	6.7	ng	77810	4	11.25	232313	20.0
5-Bromo-2-thiophe...	11.86	2.5	ng	29624	4	11.25	232313	20.0
Trichloroacetic a...	13.74	6.7	ng	110221	5	13.89	330043	20.0
2-methyloctacosane	14.34	2.6	ng	42394	5	13.89	330043	20.0
Pentacosane	14.64	3.7	ng	65042	6	15.33	352303	20.0
Benzo[e]pyrene	15.21	2.2	ng	39195	6	15.33	352303	20.0
Heneicosane	15.71	3.0	ng	53796	6	15.33	352303	20.0