

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
 Data File : BF113038.D
 Acq On : 13 Mar 2019 19:51
 Operator : JU/SJ
 Sample : K1873-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 371

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-BF022719.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF113046.D

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.345	548	554	557	rBV	3697711	3981120	80.85%	7.435%
2	6.369	723	728	733	rBV2	3603322	4448194	90.34%	8.307%
3	6.498	745	750	753	rBV	4450252	4186005	85.01%	7.817%
4	6.722	785	788	792	rBV	1060909	959228	19.48%	1.791%
5	6.881	811	815	819	rBV	3561567	3187806	64.74%	5.953%
6	7.286	879	884	887	rBV	2782612	2673196	54.29%	4.992%
7	8.004	1002	1006	1012	rBV	1290630	1206619	24.51%	2.253%
8	9.080	1185	1189	1199	rBV	4491559	4470958	90.80%	8.349%
9	9.475	1252	1256	1264	rBV	471952	415449	8.44%	0.776%
10	9.616	1276	1280	1284	rBV	84828	73388	1.49%	0.137%
11	9.757	1298	1304	1313	rBV	1395080	1362340	27.67%	2.544%
12	10.539	1433	1437	1441	rBV	3106152	3343731	67.91%	6.244%
13	10.586	1443	1445	1451	rVV	85073	122516	2.49%	0.229%
14	10.657	1454	1457	1466	rVB4	44037	76443	1.55%	0.143%
15	11.233	1551	1555	1558	rBV	1670542	1551558	31.51%	2.897%
16	11.692	1630	1633	1637	rBV4	56265	75689	1.54%	0.141%
17	11.774	1642	1647	1655	rBV2	1306099	1375245	27.93%	2.568%
18	11.839	1655	1658	1661	rBV	150839	164581	3.34%	0.307%
19	12.280	1730	1733	1736	rBV	64300	58863	1.20%	0.110%
20	12.363	1744	1747	1752	rVB2	91755	103319	2.10%	0.193%
21	12.439	1756	1760	1763	rBV	1391757	1242417	25.23%	2.320%
22	12.474	1764	1766	1773	rVB4	54656	96228	1.95%	0.180%
23	12.533	1773	1776	1777	rBV	88765	89302	1.81%	0.167%
24	12.551	1777	1779	1784	rVV	459123	409091	8.31%	0.764%
25	12.663	1792	1798	1802	rBV	1252764	1170306	23.77%	2.185%
26	12.786	1816	1819	1820	rBV	69370	65087	1.32%	0.122%
27	12.815	1820	1824	1827	rVV	4772758	4923929	100.00%	9.195%
28	12.886	1831	1836	1839	rBV3	95629	138833	2.82%	0.259%
29	12.968	1847	1850	1851	rBV	81848	72049	1.46%	0.135%
30	12.992	1851	1854	1857	rVB	243937	221419	4.50%	0.413%
31	13.057	1862	1865	1868	rVB2	206234	179654	3.65%	0.335%
32	13.098	1868	1872	1875	rBV2	127613	138056	2.80%	0.258%
33	13.186	1884	1887	1890	rVB	70282	59222	1.20%	0.111%
34	13.215	1890	1892	1897	rBV2	72190	79475	1.61%	0.148%

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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35	13.392	1920	1922	1928	rVB2	99949	118105	2.40%	0.221%
36	13.498	1937	1940	1945	rVB	79885	99389	2.02%	0.186%
37	13.604	1955	1958	1961	rBV2	92273	103255	2.10%	0.193%
38	13.633	1961	1963	1965	rVV	107083	96354	1.96%	0.180%
39	13.657	1965	1967	1972	rVV2	88590	111467	2.26%	0.208%
40	13.715	1972	1977	1984	rVB4	463507	623532	12.66%	1.164%
41	13.857	1993	2001	2004	rBV2	1795911	2286989	46.45%	4.271%
42	13.880	2004	2005	2008	rVB	497284	287840	5.85%	0.538%
43	13.998	2022	2025	2028	rBV	90811	76971	1.56%	0.144%
44	14.039	2029	2032	2035	rVB2	203365	190852	3.88%	0.356%
45	14.239	2062	2066	2069	rBV	134455	175542	3.57%	0.328%
46	14.274	2070	2072	2075	rVB	84822	79407	1.61%	0.148%
47	14.339	2079	2083	2086	rBV4	351258	363346	7.38%	0.679%
48	14.633	2130	2133	2141	rVB	393834	396742	8.06%	0.741%
49	14.704	2141	2145	2150	rBV2	353843	357904	7.27%	0.668%
50	14.862	2168	2172	2175	rBV	532628	770253	15.64%	1.438%
51	14.951	2183	2187	2194	rVB2	372541	524757	10.66%	0.980%
52	15.145	2216	2220	2225	rVB	303991	374221	7.60%	0.699%
53	15.198	2225	2229	2235	rBV	430331	541693	11.00%	1.012%
54	15.262	2235	2240	2243	rBV	1094533	1296955	26.34%	2.422%
55	15.304	2243	2247	2252	rVB2	337526	503812	10.23%	0.941%
56	15.704	2311	2315	2320	rBV	275723	430815	8.75%	0.805%
57	16.168	2390	2394	2398	rBV	166789	274492	5.57%	0.513%
58	16.609	2464	2469	2479	rVB2	206347	423442	8.60%	0.791%
59	17.015	2533	2538	2548	rVB	164215	319745	6.49%	0.597%

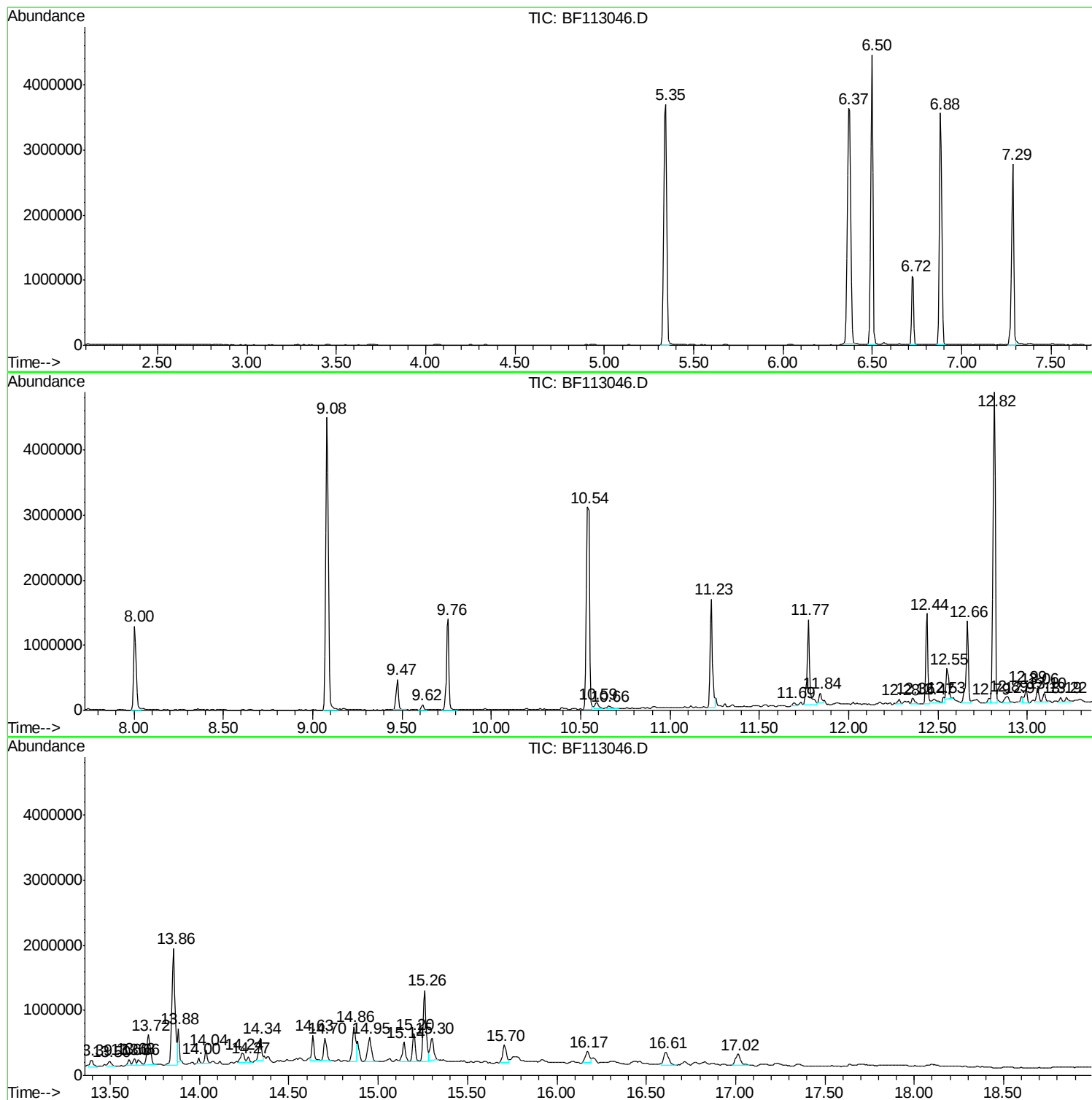
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampleId :
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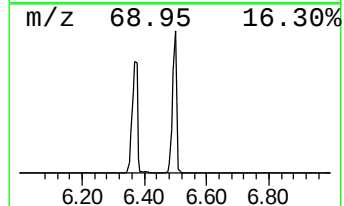
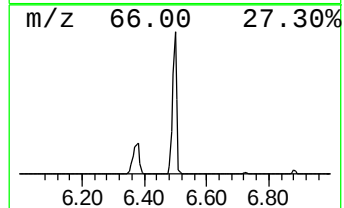
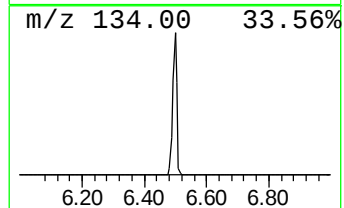
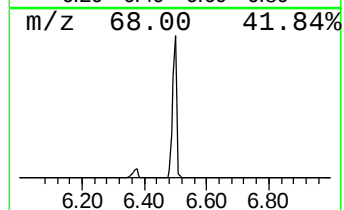
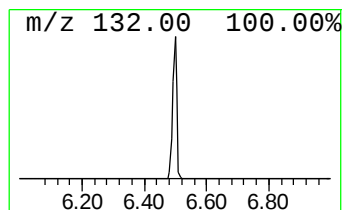
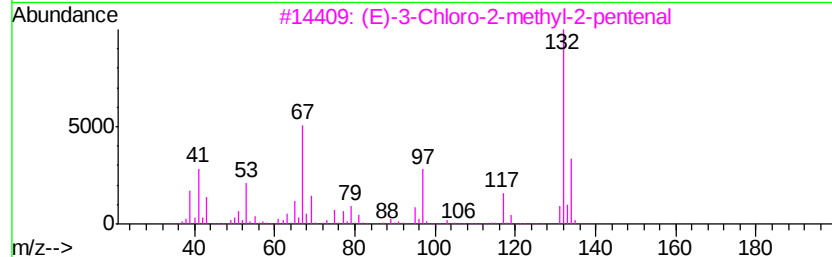
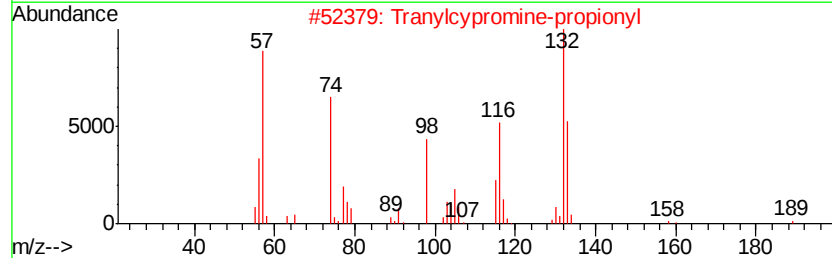
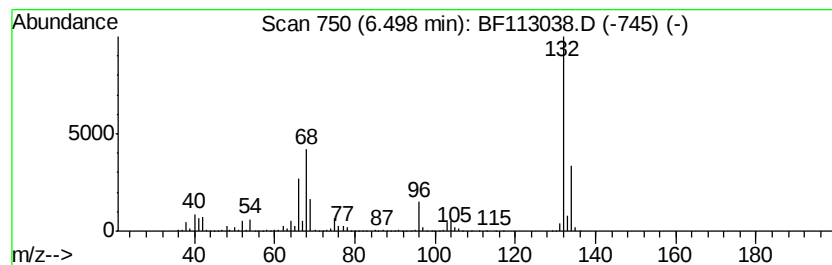
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	87.28 ng	4186010	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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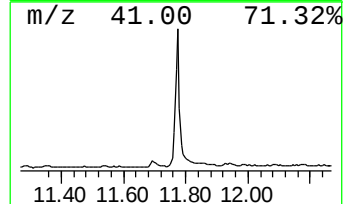
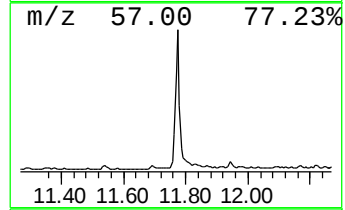
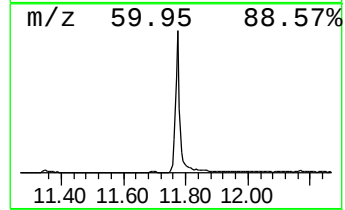
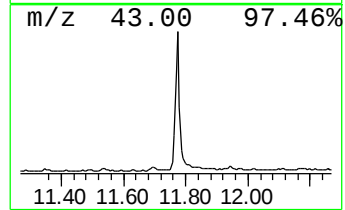
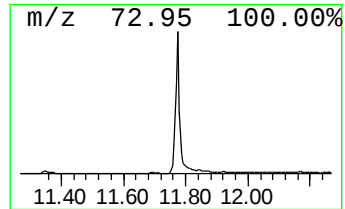
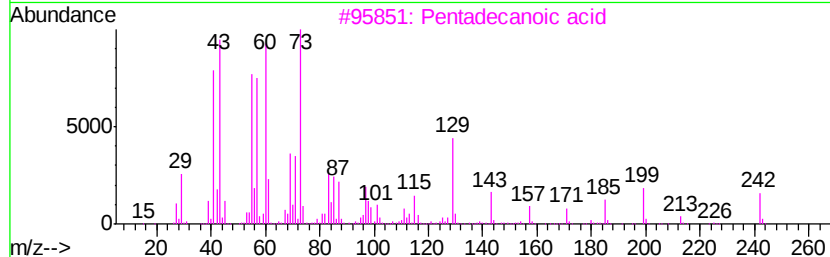
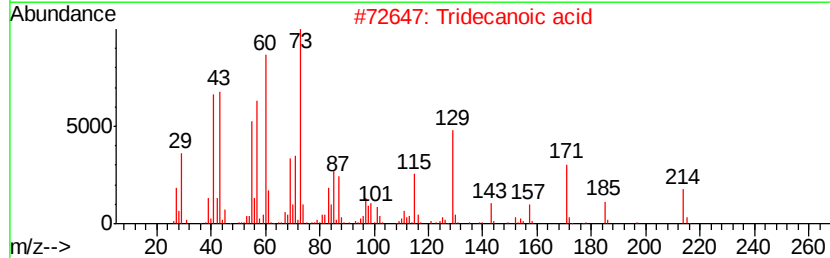
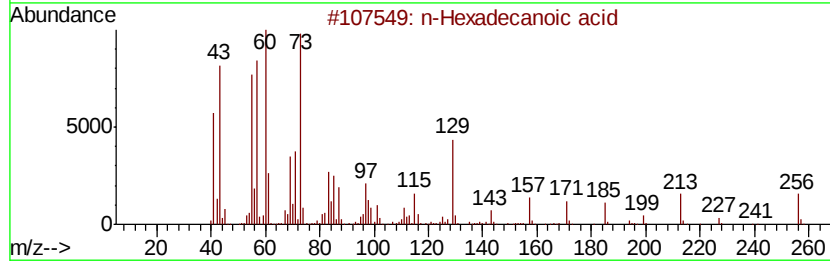
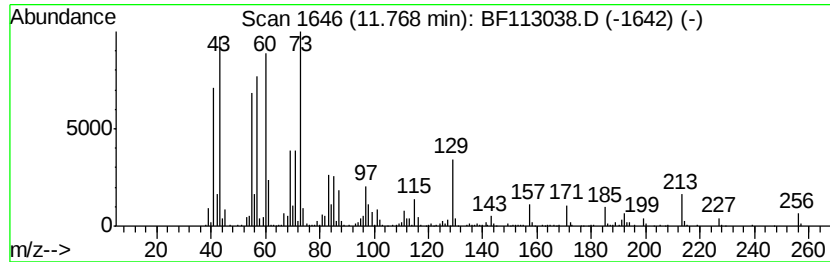
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	17.73 ng	1375250	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	95
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4		Octadecanoic acid	284	C18H36O2	000057-11-4	90
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	87



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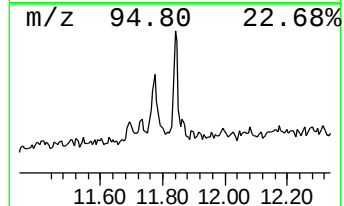
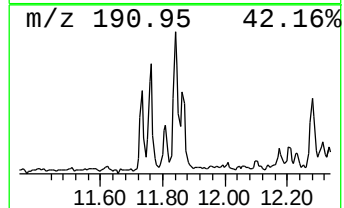
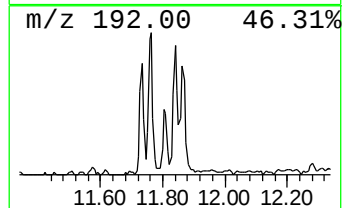
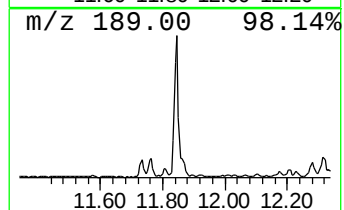
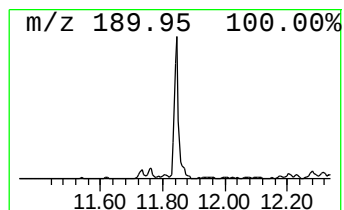
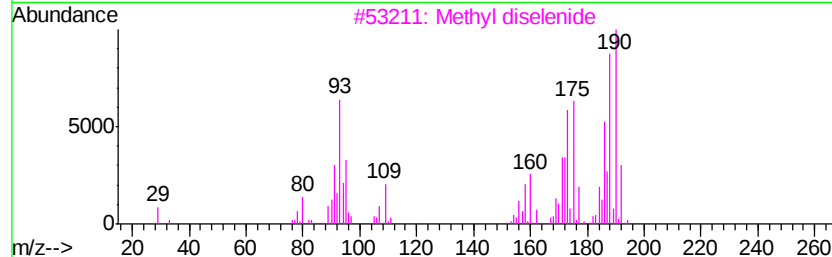
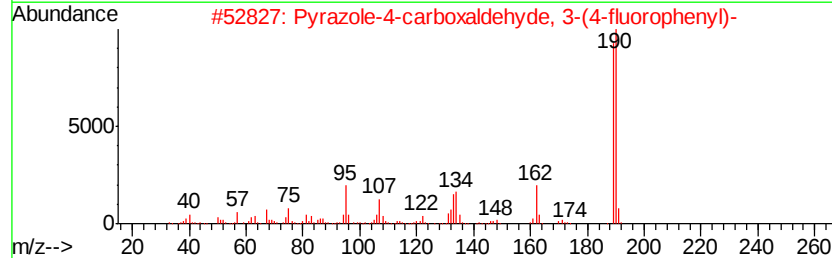
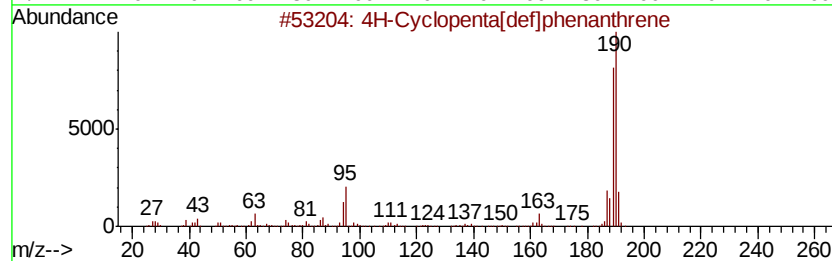
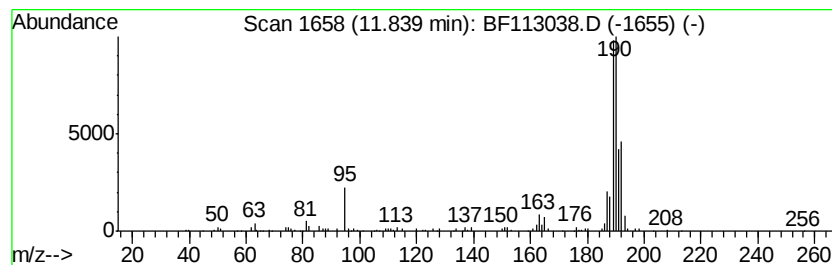
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.12 ng	164581	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2		Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	49
3		Methyl diselenide	190	C2H6Se2	007101-31-7	43
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
5		Benzo[1,2-b:4,3-b']dithiophene	190	C10H6S2	000210-80-0	12



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Misc :
ALS Vial : 8 Sample Multiplier: 1

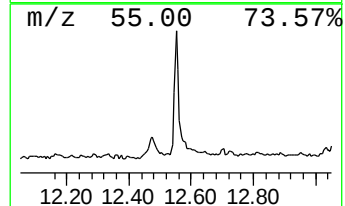
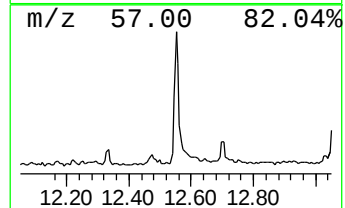
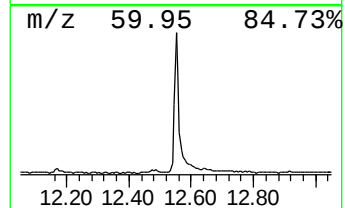
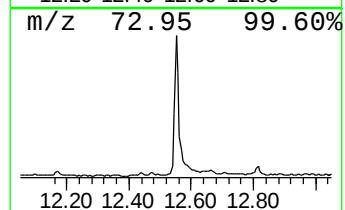
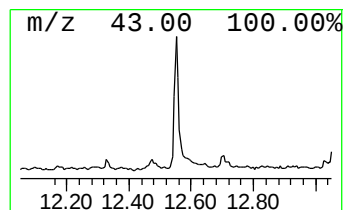
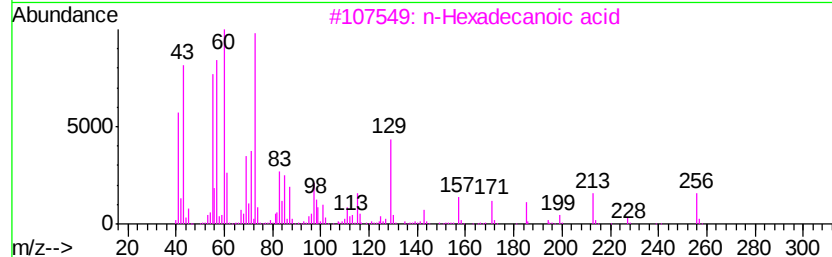
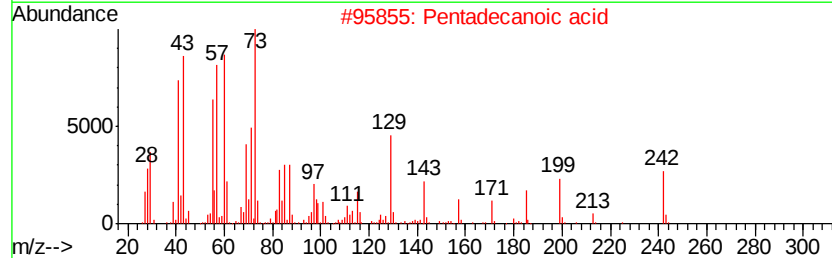
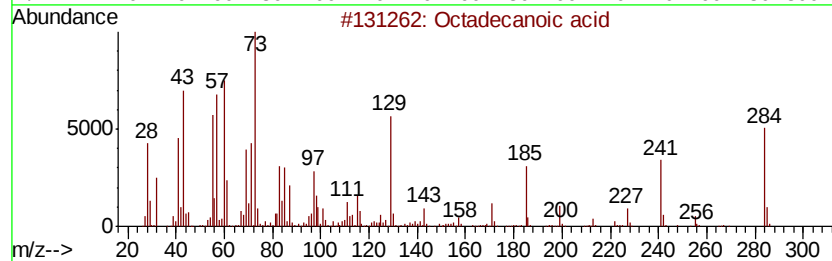
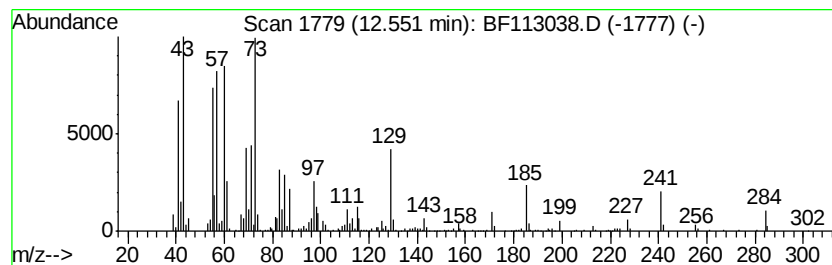
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.55	3.58 ng	409091	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	62



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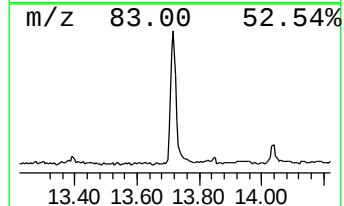
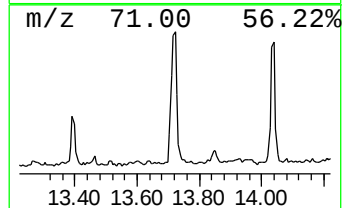
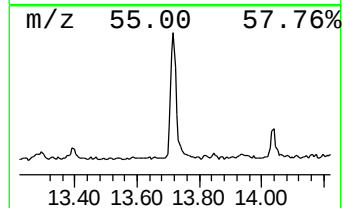
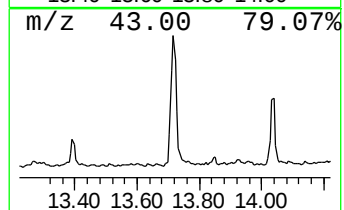
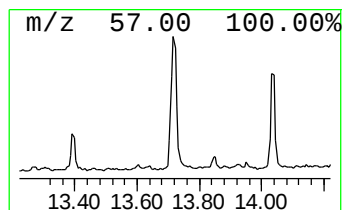
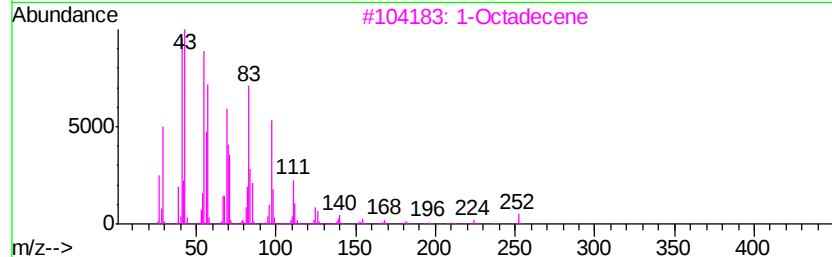
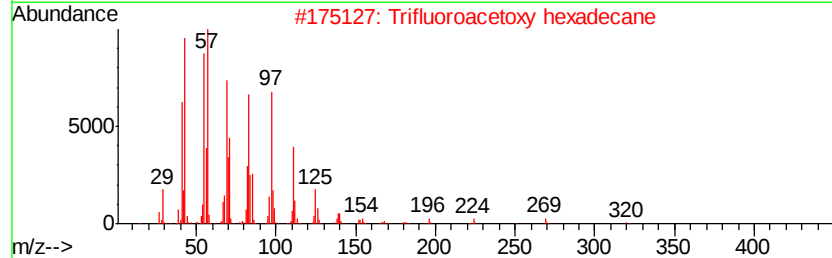
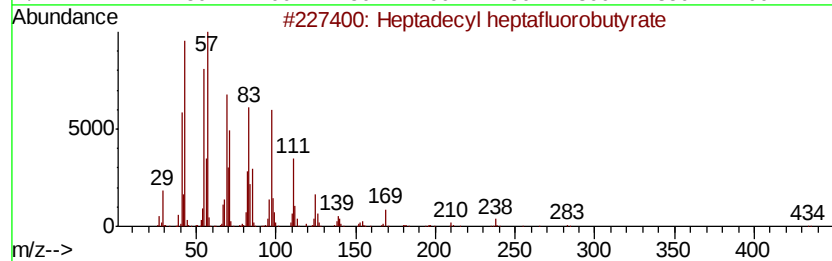
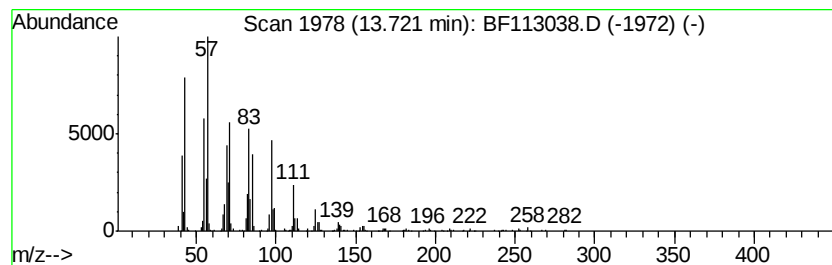
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.45 ng	623532	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		1-Octadecene	252	C18H36	000112-88-9	93
4		1-Heneicosanol	312	C21H44O	015594-90-8	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
 Data File : BF113038.D
 Acq On : 13 Mar 2019 19:51
 Operator : JU/SJ
 Sample : K1873-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

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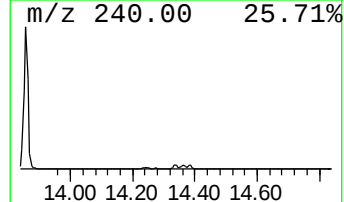
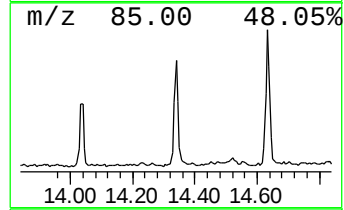
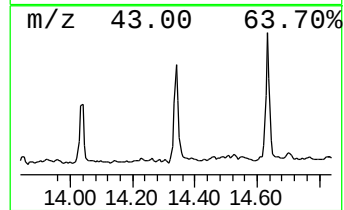
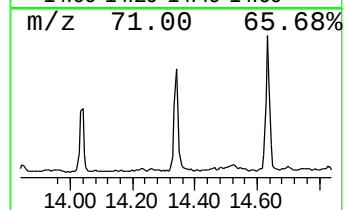
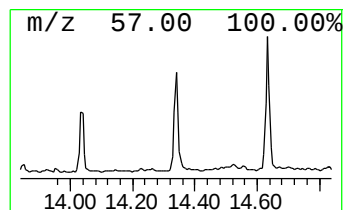
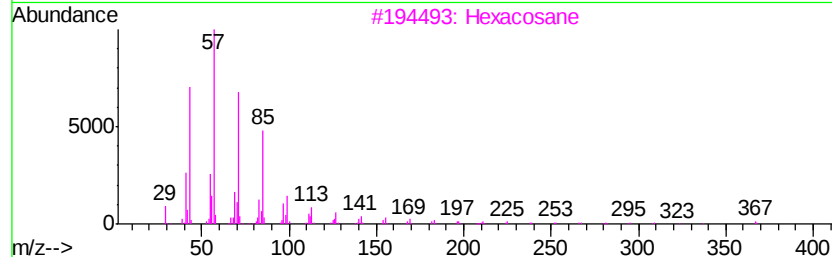
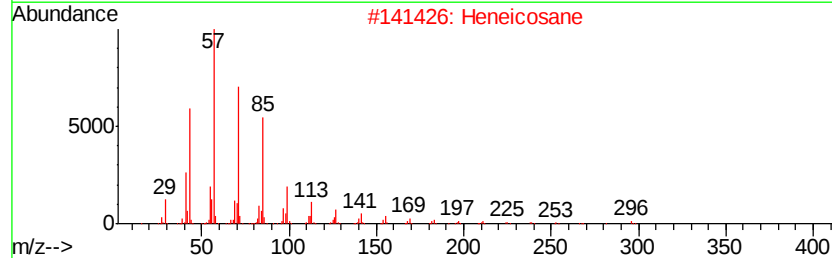
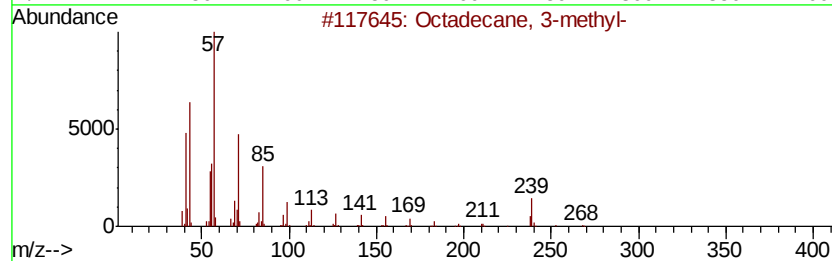
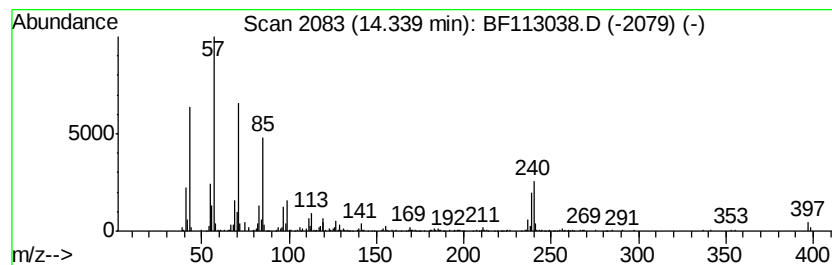
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 7 Octadecane, 3-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	3.18 ng	363346	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane, 3-methyl-	268	C19H40	006561-44-0	68
2		Heneicosane	296	C21H44	000629-94-7	64
3		Hexacosane	366	C26H54	000630-01-3	64
4		Octacosane	394	C28H58	000630-02-4	64
5		Nonadecane, 4-methyl-	282	C20H42	025117-27-5	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
Data File : BF113038.D
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Sample : K1873-01
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Instrument :
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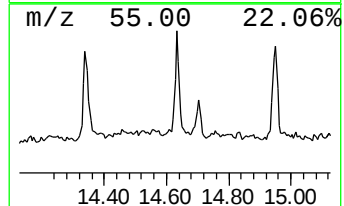
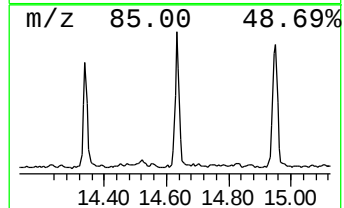
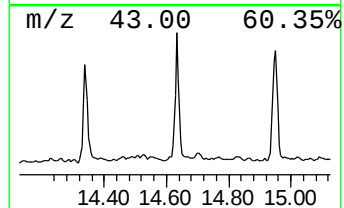
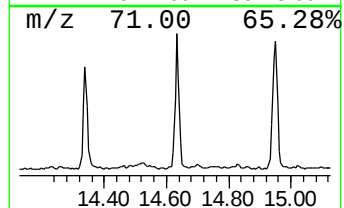
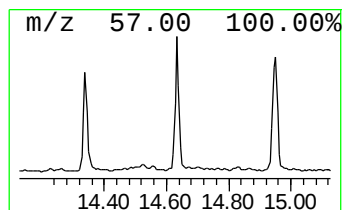
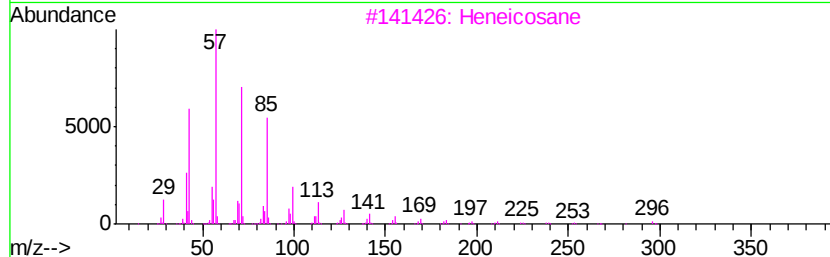
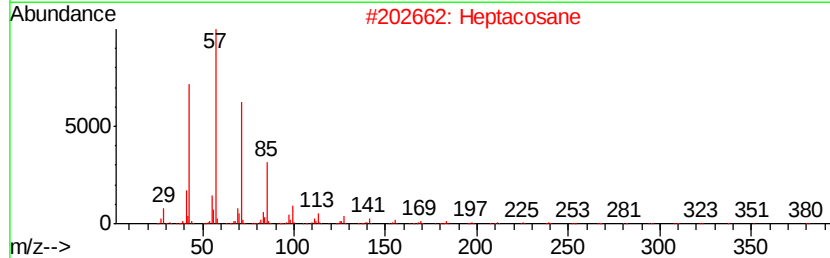
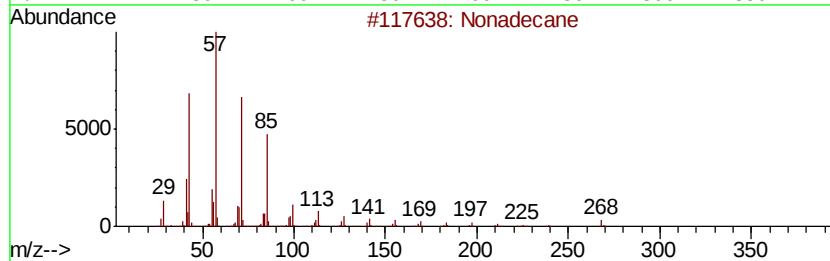
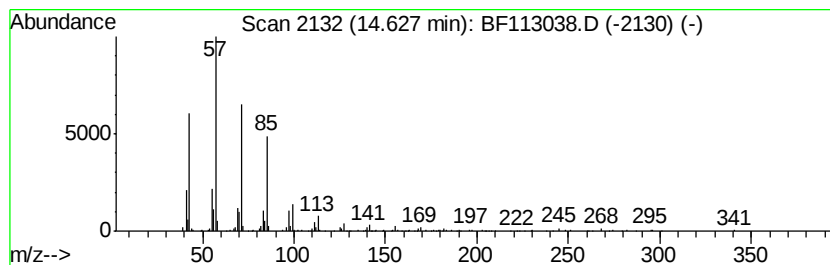
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	6.12 ng	396742	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	95
2	Heptacosane		380	C27H56	000593-49-7	87
3	Heneicosane		296	C21H44	000629-94-7	87
4	Decane, 3,8-dimethyl-		170	C12H26	017312-55-9	87
5	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	86



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Sample : K1873-01
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ALS Vial : 8 Sample Multiplier: 1

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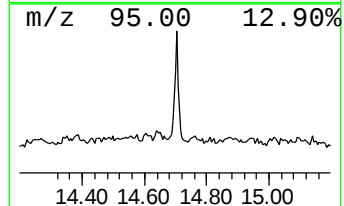
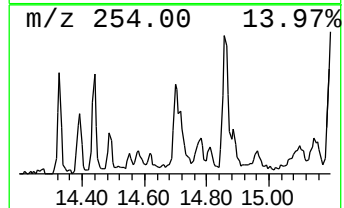
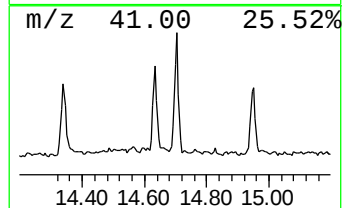
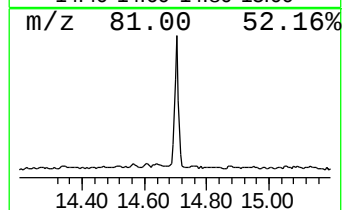
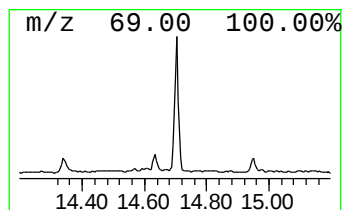
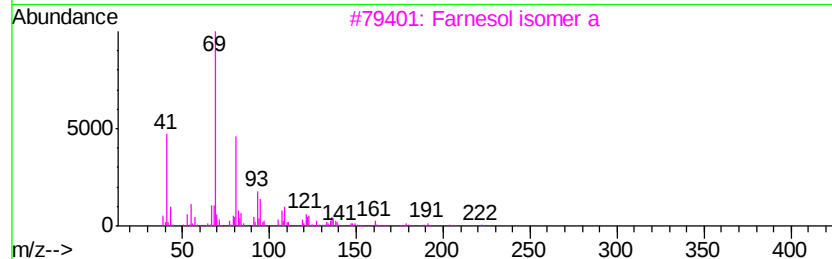
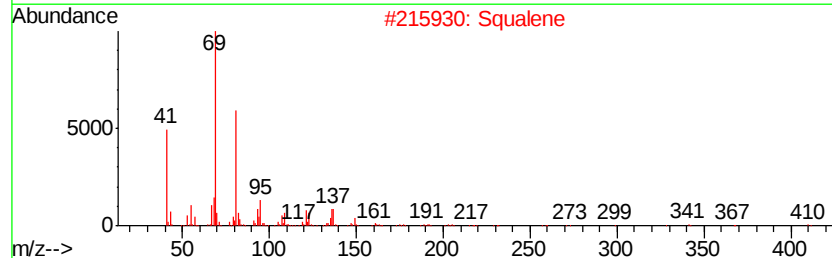
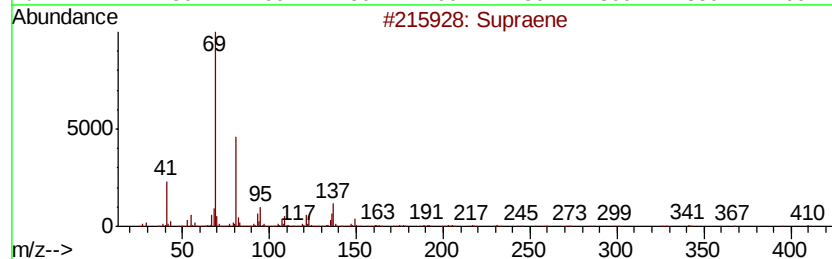
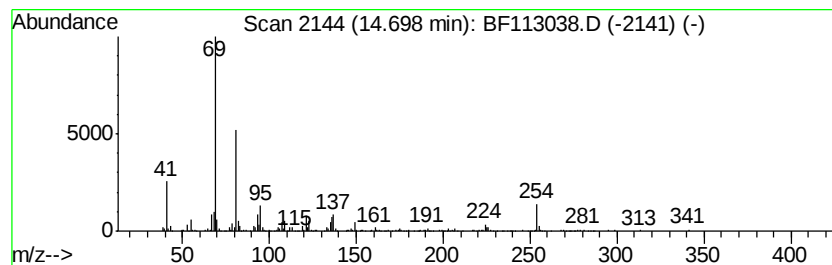
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	5.52 ng	357904	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	90
2	Squalene		410	C30H50	000111-02-4	90
3	Farnesol isomer a		222	C15H26O	1000108-92-4	76
4	2,6-Octadiene, 4-methyl-		124	C9H16	074498-94-5	50
5	4-Methyl-1,5-Heptadiene		110	C8H14	000998-94-7	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF031319\
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Sample : K1873-01
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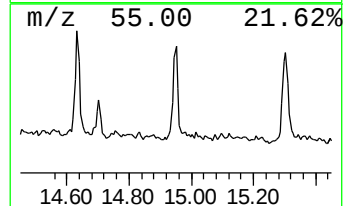
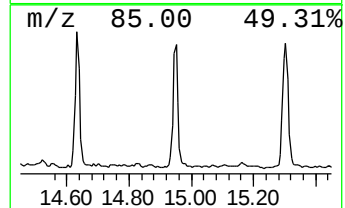
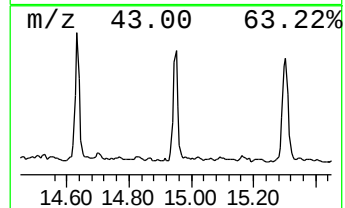
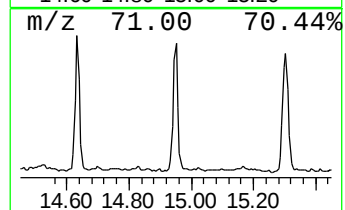
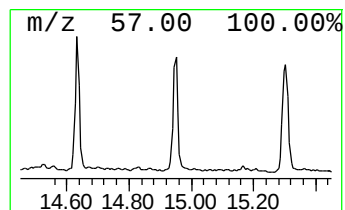
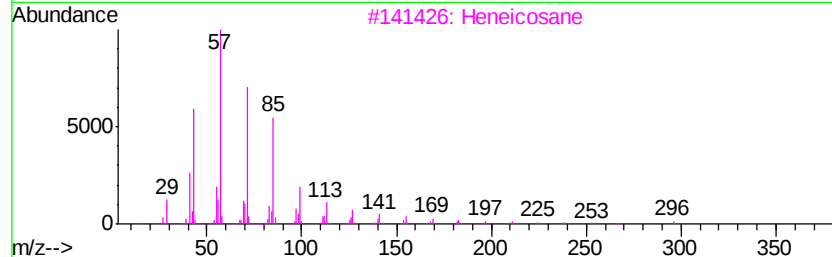
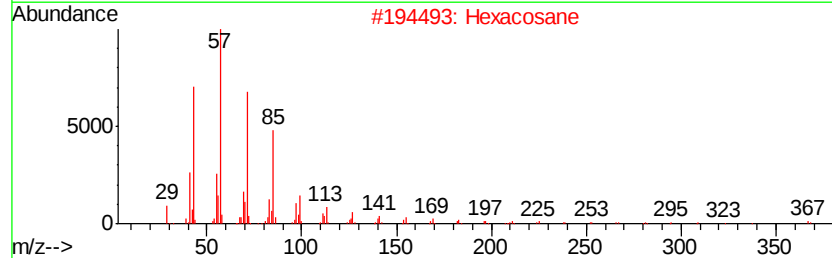
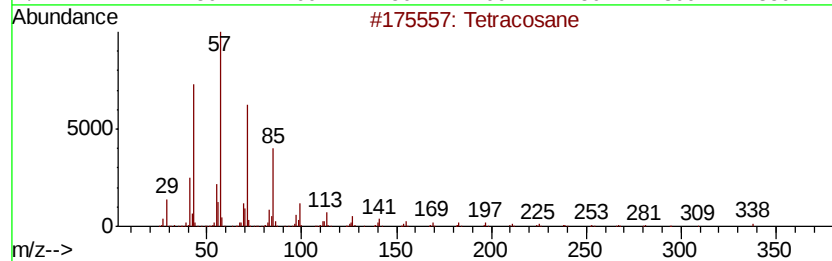
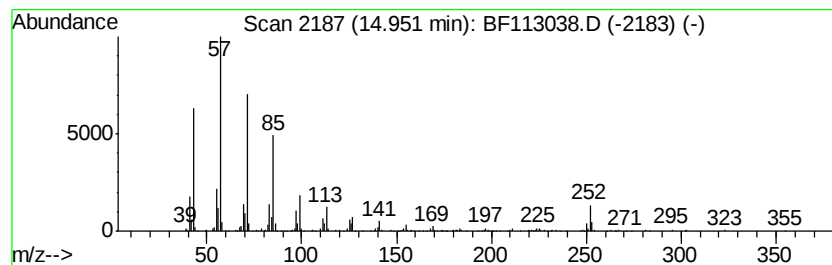
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	8.09 ng	524757	Perylene-d12	15.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetracosane	338	C24H50	000646-31-1	87
2		Hexacosane	366	C26H54	000630-01-3	87
3		Heneicosane	296	C21H44	000629-94-7	87
4		2-methyloctacosane	408	C29H60	1000376-72-8	83
5		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	80



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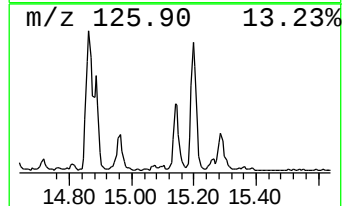
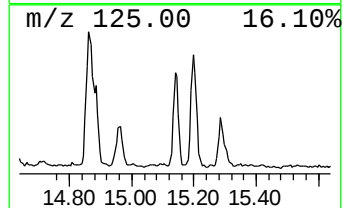
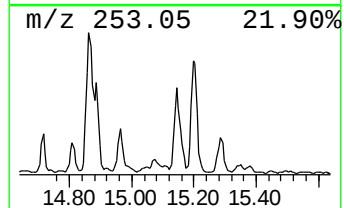
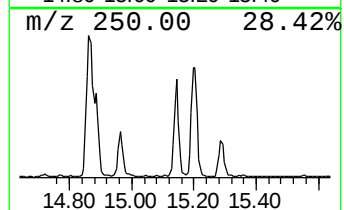
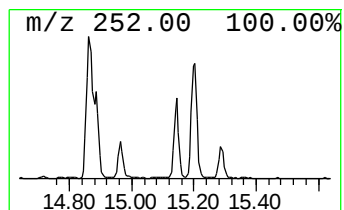
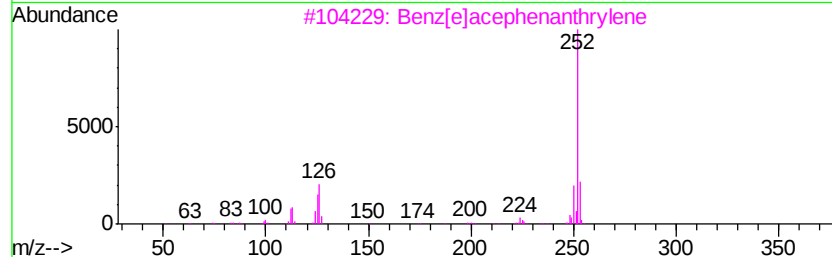
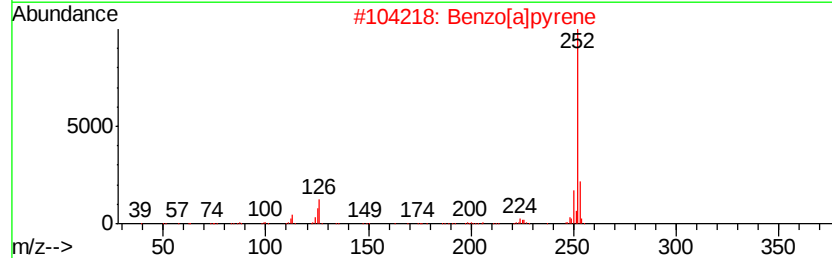
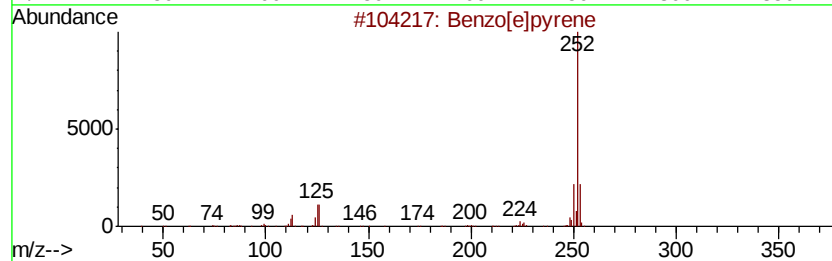
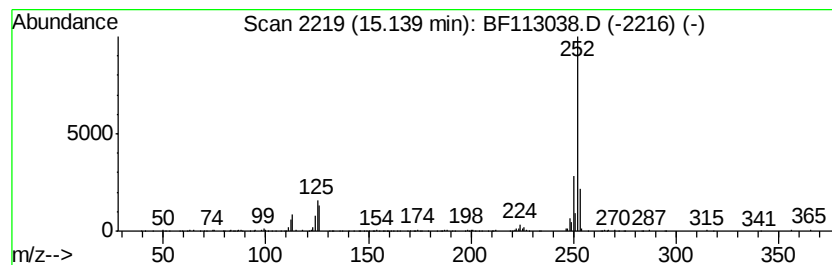
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.14	5.77 ng	374221	Perylene-d12	15.26

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	96
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4			Perylene	252	C20H12	000198-55-0	95
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	91



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Sample : K1873-01
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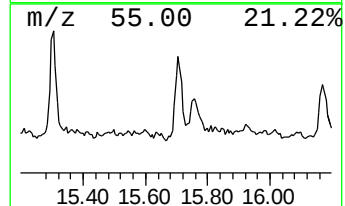
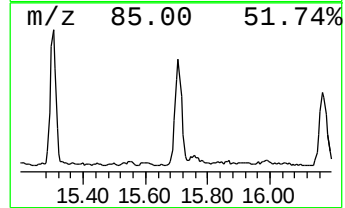
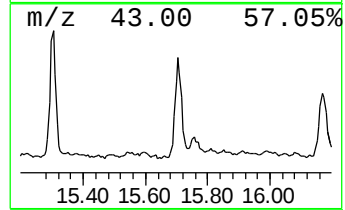
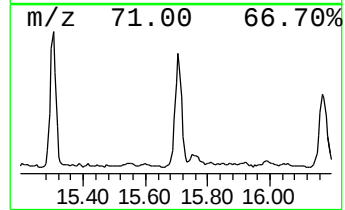
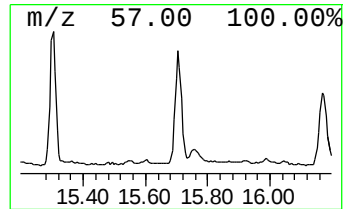
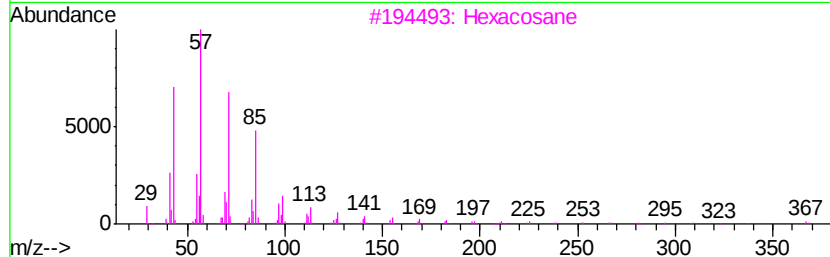
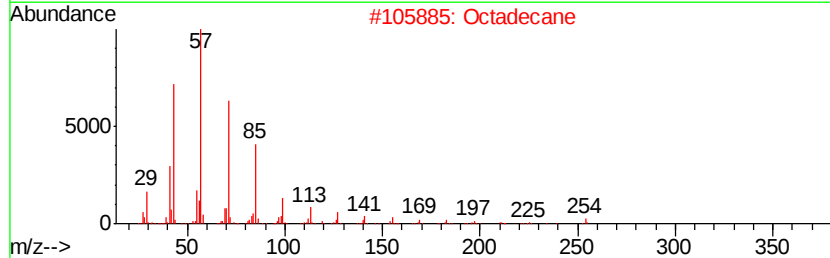
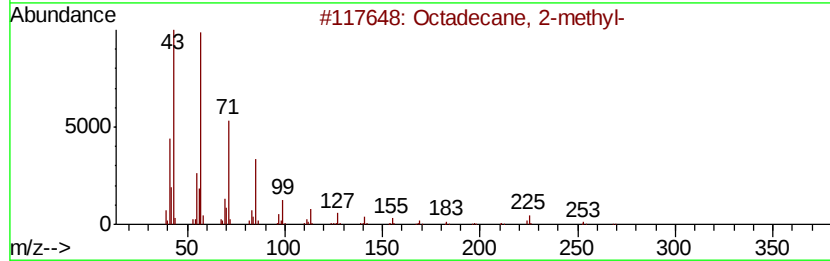
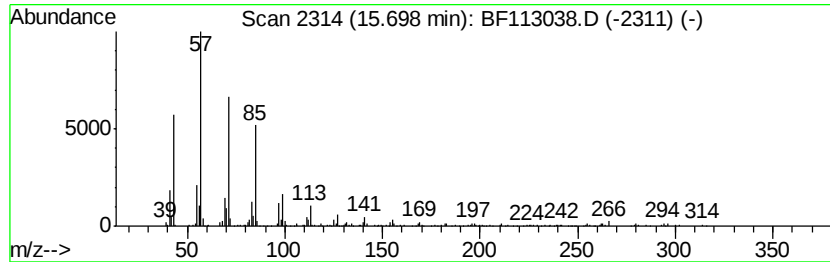
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	6.64 ng	430815	Perylene-d12	15.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
2			Octadecane	254	C18H38	000593-45-3	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Heneicosane	296	C21H44	000629-94-7	90
5			triacontane	422	C30H62	000638-68-6	87



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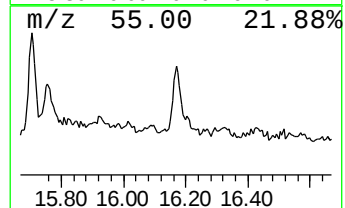
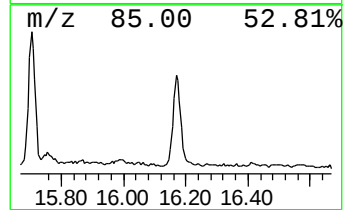
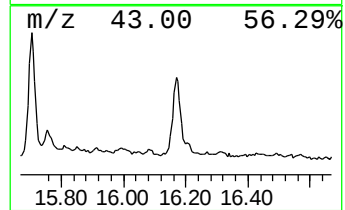
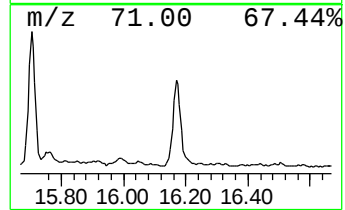
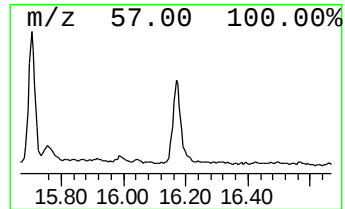
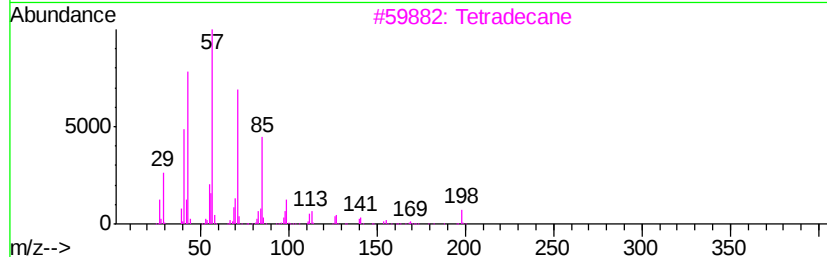
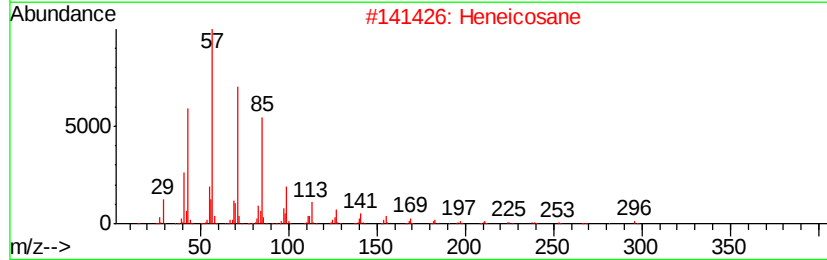
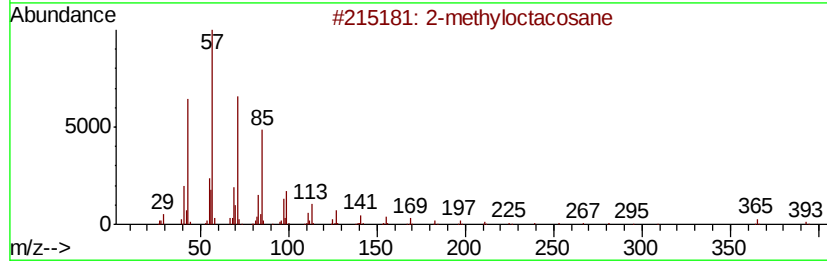
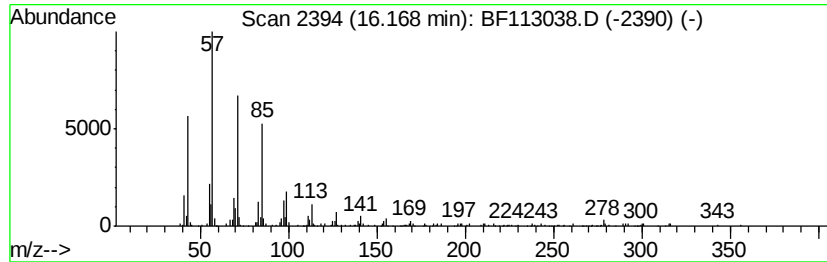
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	4.23 ng	274492	Perylene-d12	15.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	90
2		Heneicosane	296	C21H44	000629-94-7	87
3		Tetradecane	198	C14H30	000629-59-4	87
4		Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF031319\
Data File : BF113038.D
Acq On : 13 Mar 2019 19:51
Operator : JU/SJ
Sample : K1873-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
371

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	87.3	ng	4186010	1	6.73	959228	20.0
n-Hexadecanoic acid	11.77	17.7	ng	1375250	4	11.23	1551560	20.0
4H-Cyclopenta[def...	11.84	2.1	ng	164581	4	11.23	1551560	20.0
Octadecanoic acid	12.55	3.6	ng	409091	5	13.86	2286990	20.0
Heptadecyl hepta...	13.72	5.5	ng	623532	5	13.86	2286990	20.0
Octadecane, 3-met...	14.34	3.2	ng	363346	5	13.86	2286990	20.0
Nonadecane	14.63	6.1	ng	396742	6	15.26	1296960	20.0
Supraene	14.70	5.5	ng	357904	6	15.26	1296960	20.0
Tetracosane	14.95	8.1	ng	524757	6	15.26	1296960	20.0
Benzo[e]pyrene	15.14	5.8	ng	374221	6	15.26	1296960	20.0
Octadecane, 2-met...	15.70	6.6	ng	430815	6	15.26	1296960	20.0
2-methyloctacosane	16.17	4.2	ng	274492	6	15.26	1296960	20.0