

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
 Data File : BF097891.D
 Acq On : 19 Aug 2017 21:00
 Operator : SJ/JU
 Sample : I4845-01 10X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OK-03-81617

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:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	482	485	490	rVB	45443	47245	3.87%	0.425%
2	5.357	552	556	561	rVB	339182	316852	25.97%	2.849%
3	6.381	727	730	738	rBV	428645	341822	28.02%	3.074%
4	6.522	750	754	761	rVB	442517	350774	28.75%	3.154%
5	6.757	791	794	798	rBV	1048661	961579	78.81%	8.647%
6	6.916	817	821	824	rBV	309609	264416	21.67%	2.378%
7	7.316	883	889	893	rBV	247929	207092	16.97%	1.862%
8	8.045	1008	1013	1016	rBV	1437907	1220061	100.00%	10.971%
9	8.339	1056	1063	1066	rBV5	12139	20662	1.69%	0.186%
10	8.469	1081	1085	1087	rBV	16172	14950	1.23%	0.134%
11	8.545	1094	1098	1101	rBV2	19720	19802	1.62%	0.178%
12	8.639	1111	1114	1117	rBV	45559	38006	3.12%	0.342%
13	8.869	1147	1153	1155	rBV3	20518	25657	2.10%	0.231%
14	9.069	1184	1187	1191	rVB3	22562	24469	2.01%	0.220%
15	9.116	1191	1195	1200	rBV	491222	387024	31.72%	3.480%
16	9.204	1206	1210	1215	rBV	68616	64164	5.26%	0.577%
17	9.510	1259	1262	1266	rBV2	54647	74604	6.11%	0.671%
18	9.545	1266	1268	1271	rVV4	21120	19613	1.61%	0.176%
19	9.580	1271	1274	1277	rVB3	17090	16039	1.31%	0.144%
20	9.733	1297	1300	1304	rVB	86275	65708	5.39%	0.591%
21	9.792	1304	1310	1314	rBV	1207888	1160457	95.11%	10.435%
22	9.969	1335	1340	1342	rBV6	13192	23126	1.90%	0.208%
23	10.057	1352	1355	1358	rVB3	18547	17105	1.40%	0.154%
24	10.233	1382	1385	1387	rVB	95054	75411	6.18%	0.678%
25	10.451	1416	1422	1428	rBV	45486	62122	5.09%	0.559%
26	10.533	1434	1436	1439	rBV3	14740	15935	1.31%	0.143%
27	10.574	1439	1443	1447	rVV	179546	153523	12.58%	1.380%
28	10.704	1462	1465	1474	rBV	131648	141213	11.57%	1.270%
29	11.027	1518	1520	1526	rVB5	14318	17850	1.46%	0.161%
30	11.151	1538	1541	1543	rBV	112558	82508	6.76%	0.742%
31	11.180	1543	1546	1552	rVB	49566	54967	4.51%	0.494%
32	11.274	1558	1562	1568	rBV	1085127	937300	76.82%	8.428%
33	11.333	1568	1572	1576	rBV6	9517	16366	1.34%	0.147%
34	11.510	1596	1602	1604	rBV7	12102	23969	1.96%	0.216%

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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	11.580	1610	1614	1616	rBV	79805	71385	5.85%	0.642%
36	11.674	1627	1630	1635	rVB	198846	173087	14.19%	1.556%
37	11.886	1661	1666	1668	rBV5	17117	28381	2.33%	0.255%
38	11.986	1680	1683	1685	rBV	80436	71970	5.90%	0.647%
39	12.139	1706	1709	1711	rBV3	11545	13910	1.14%	0.125%
40	12.327	1738	1741	1743	rBV3	42797	41685	3.42%	0.375%
41	12.363	1743	1747	1749	rVV	699544	696975	57.13%	6.267%
42	12.380	1749	1750	1758	rVB2	434993	344185	28.21%	3.095%
43	12.468	1762	1765	1770	rVB2	88796	92056	7.55%	0.828%
44	12.710	1804	1806	1809	rBV	30728	23151	1.90%	0.208%
45	12.745	1809	1812	1815	rVB	78293	62280	5.10%	0.560%
46	12.857	1827	1831	1835	rBV	315072	268860	22.04%	2.418%
47	13.039	1860	1862	1865	rBV4	18738	15447	1.27%	0.139%
48	13.098	1869	1872	1876	rVV	76576	71414	5.85%	0.642%
49	13.221	1891	1893	1897	rBV4	16223	21272	1.74%	0.191%
50	13.304	1904	1907	1911	rBV5	28543	37309	3.06%	0.335%
51	13.439	1927	1930	1934	rBV	74180	76779	6.29%	0.690%
52	13.768	1983	1986	1991	rVB	96186	94772	7.77%	0.852%
53	13.904	2005	2009	2013	rBV	822310	777488	63.73%	6.991%
54	14.086	2037	2040	2043	rVB	79457	74023	6.07%	0.666%
55	14.392	2089	2092	2095	rBV	86918	93205	7.64%	0.838%
56	14.692	2140	2143	2149	rBV3	70379	84826	6.95%	0.763%
57	15.015	2195	2198	2205	rVB	81106	94575	7.75%	0.850%
58	15.333	2247	2252	2256	rBV	440602	529545	43.40%	4.762%

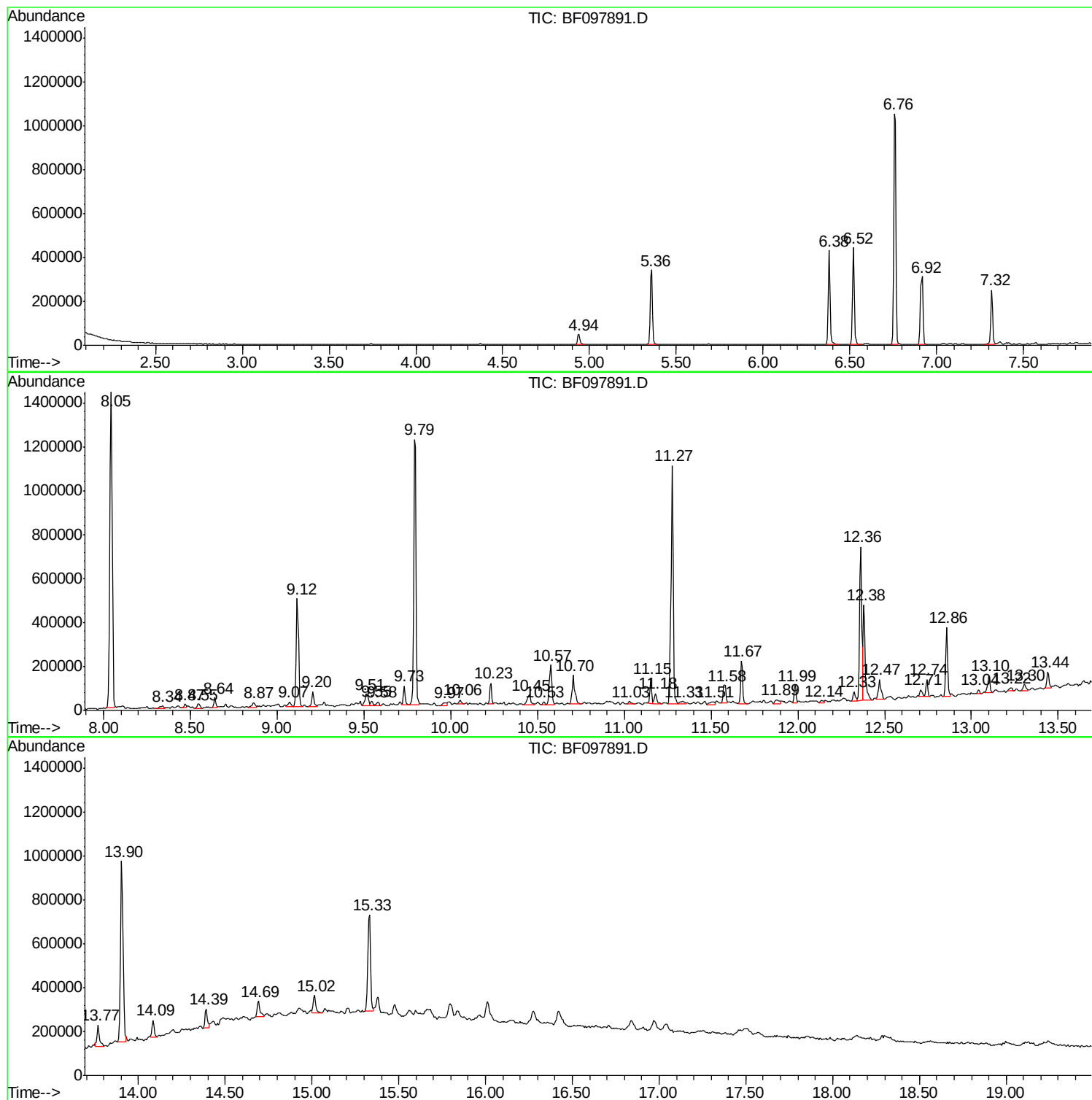
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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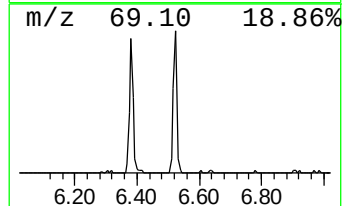
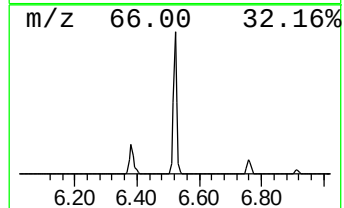
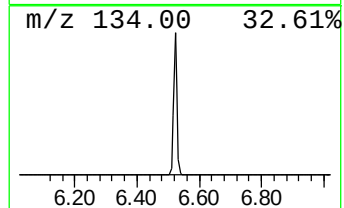
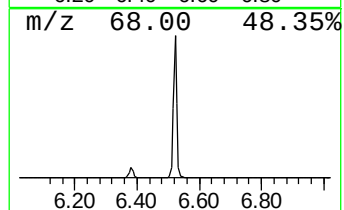
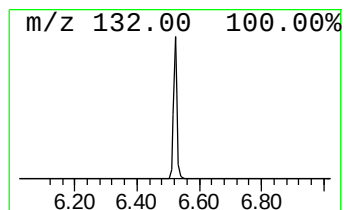
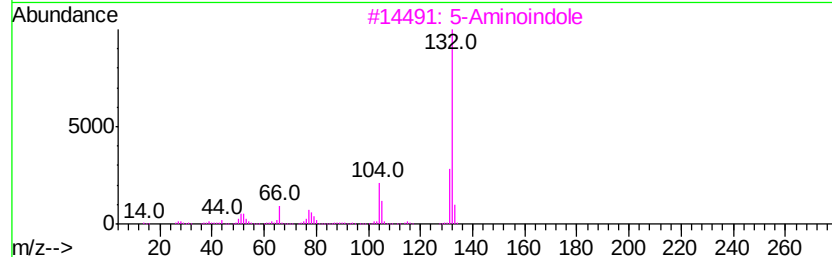
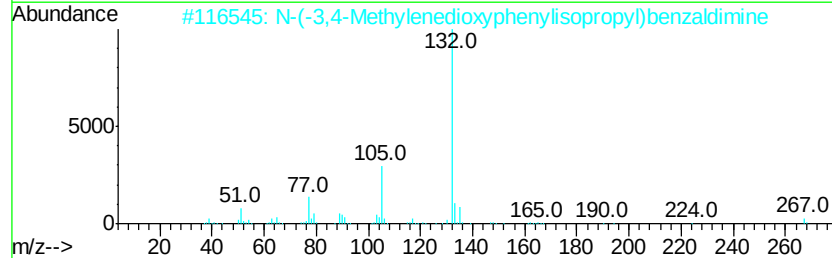
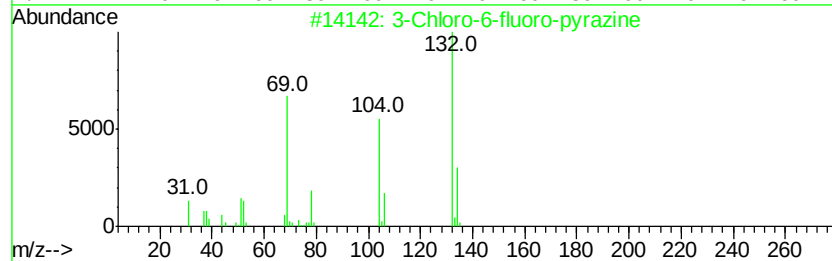
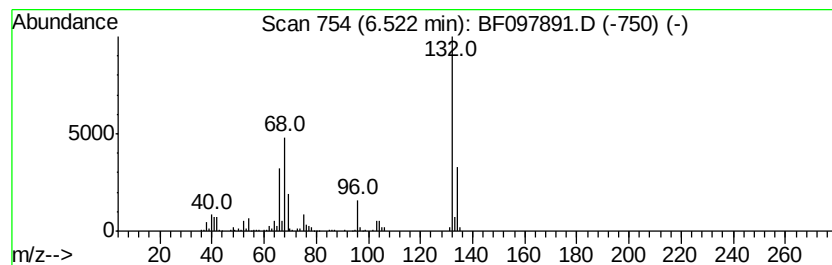
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	7.30 ng	350774	1,4-Dichlorobenzene-d4	6.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		N-(-3,4-Methylenedioxyphenylisopropyl)benzaldimine	267	C17H17NO2	1000378-96-6	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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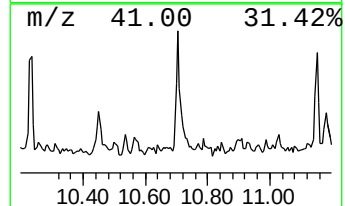
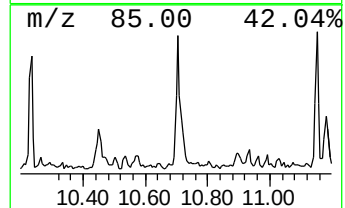
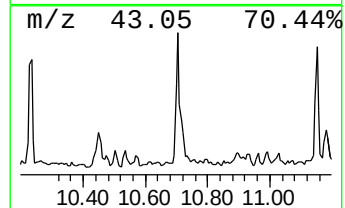
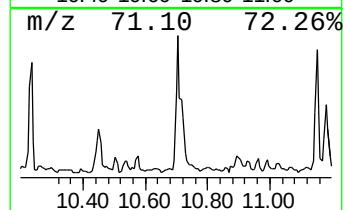
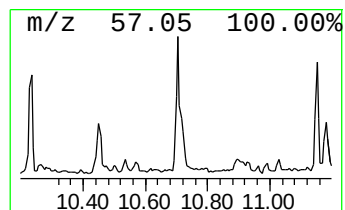
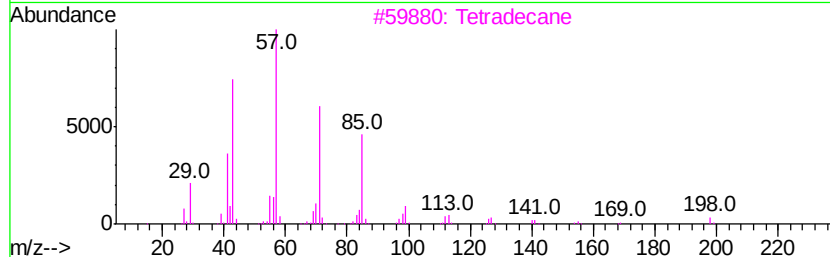
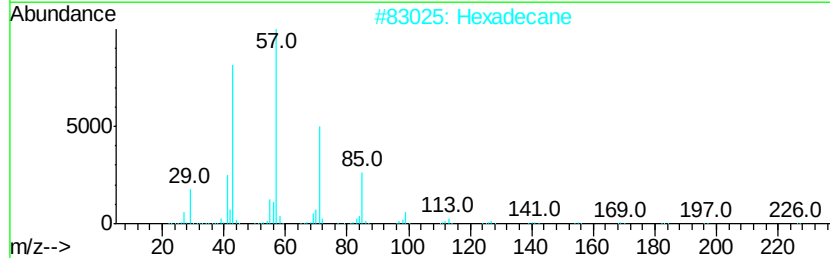
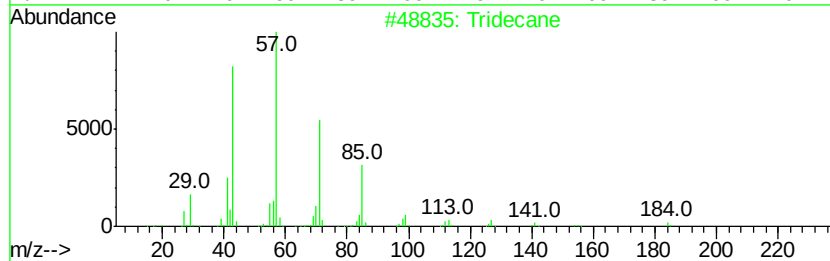
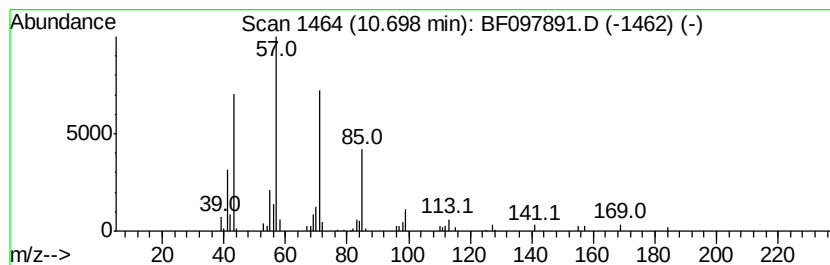
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Tridecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.70	3.01 ng	141213	Phenanthrene-d10		11.27
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	94
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetradecane	198	C14H30	000629-59-4	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Heptacosane	380	C27H56	000593-49-7	87



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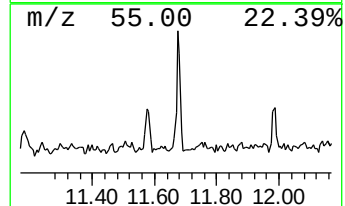
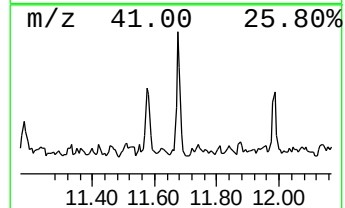
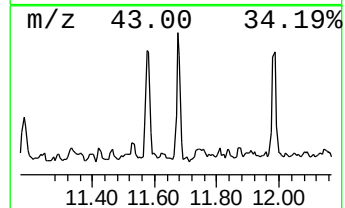
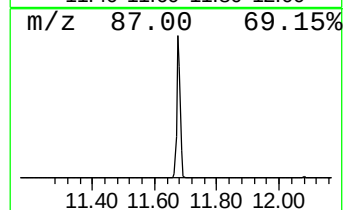
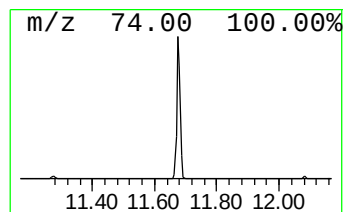
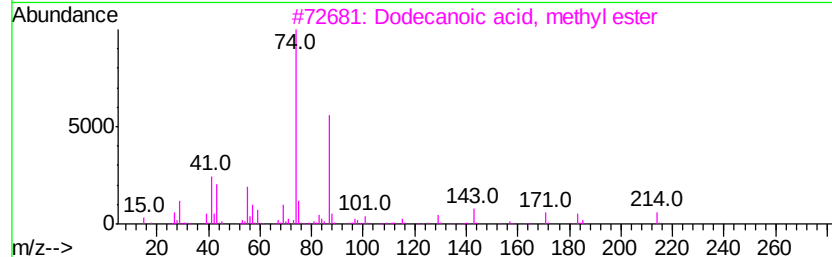
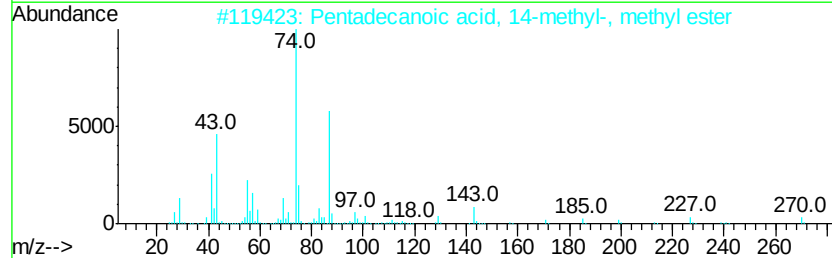
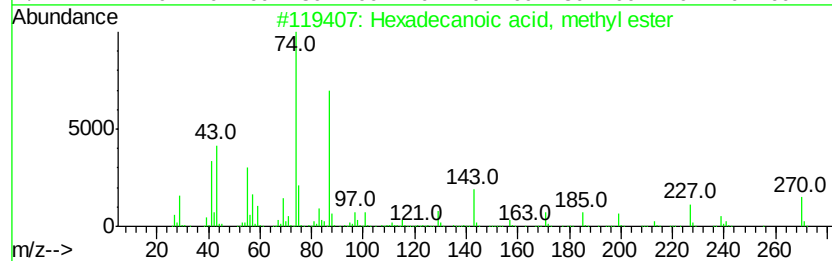
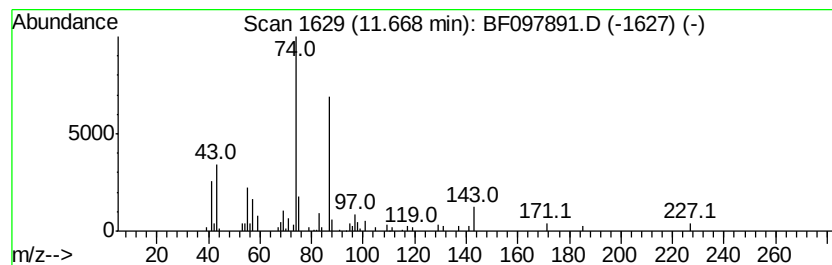
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.67	3.69 ng	173087	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	90
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
5	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90



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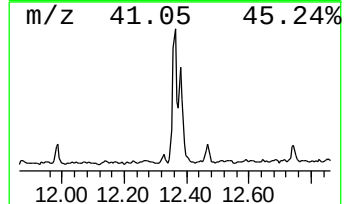
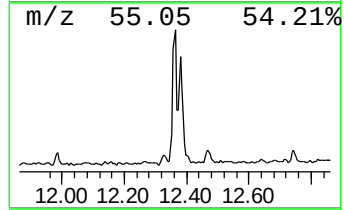
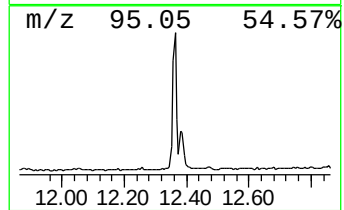
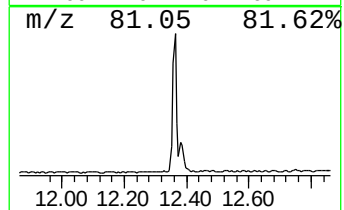
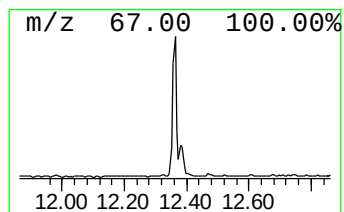
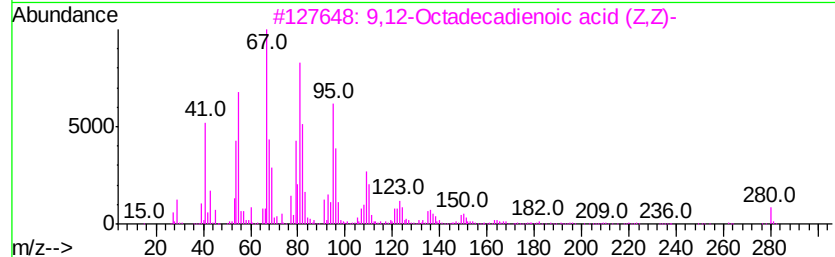
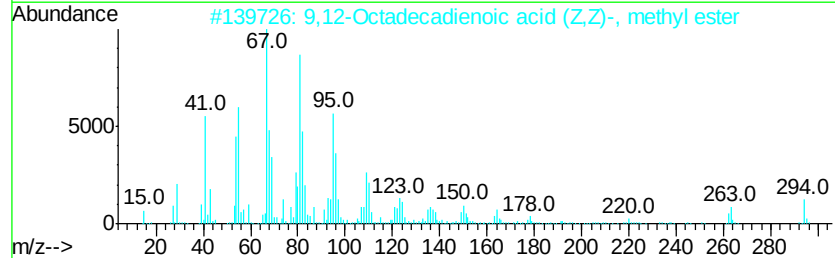
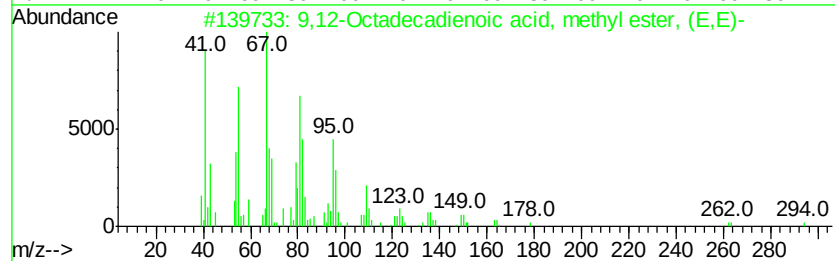
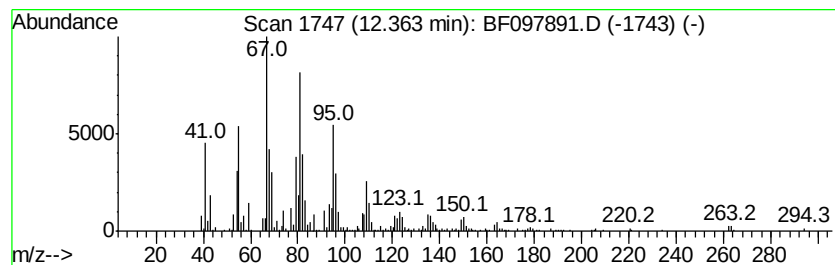
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	14.87 ng	696975	Phenanthrene-d10	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2		9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3		9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
4		9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	89
5		2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	87



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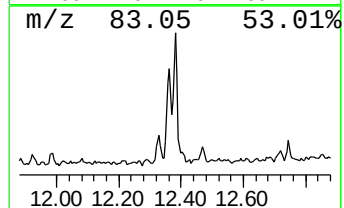
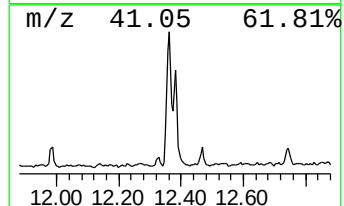
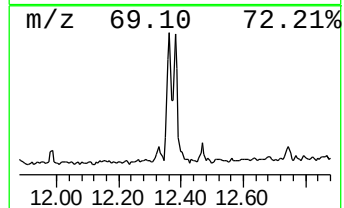
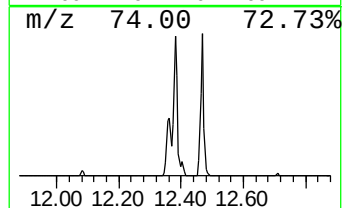
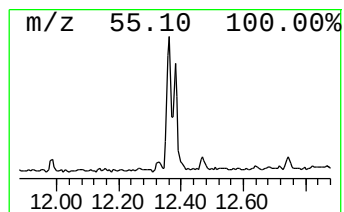
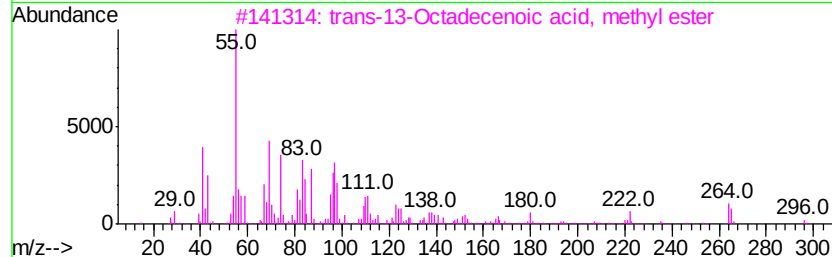
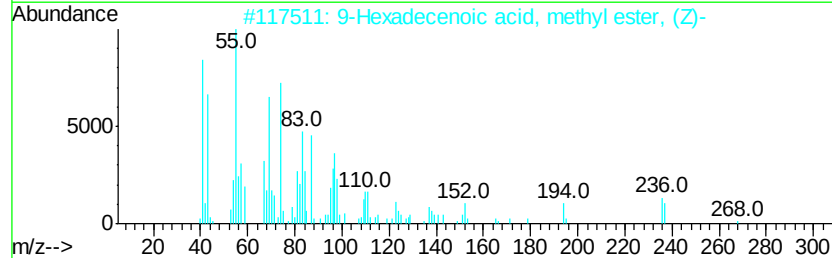
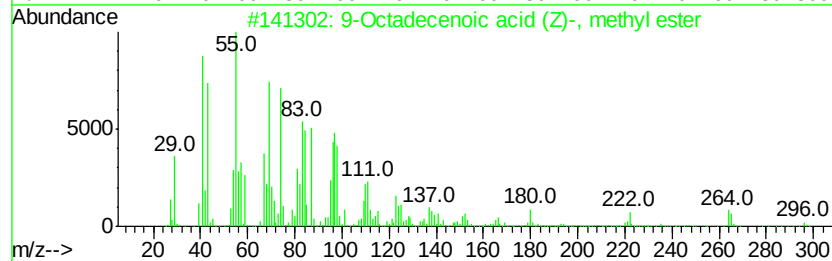
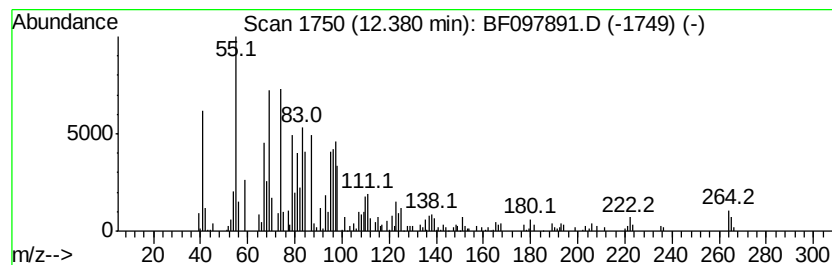
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.38	7.34 ng	344185	Phenanthrene-d10	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2		9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	81
3		trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	74
4		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	74
5		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	74



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097891.D
Acq On : 19 Aug 2017 21:00
Operator : SJ/JU
Sample : I4845-01 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-81617

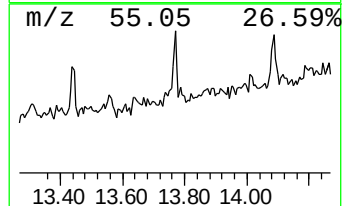
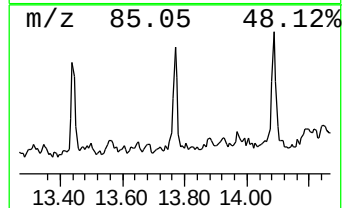
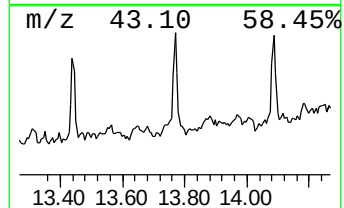
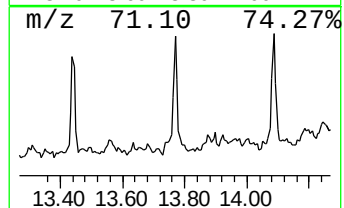
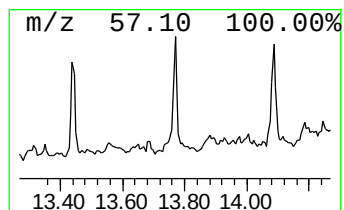
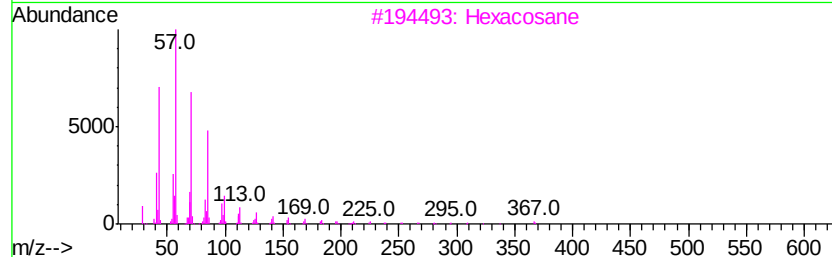
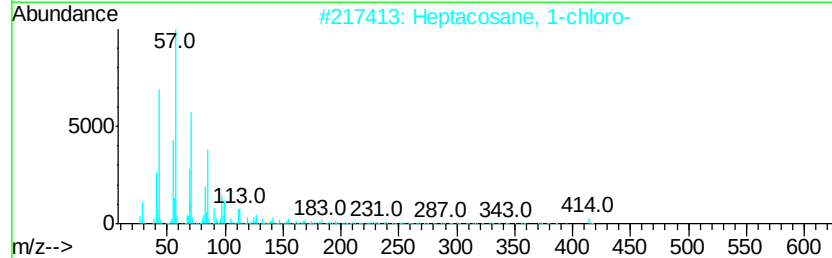
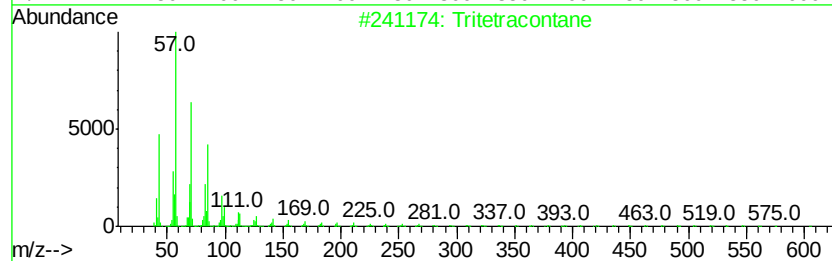
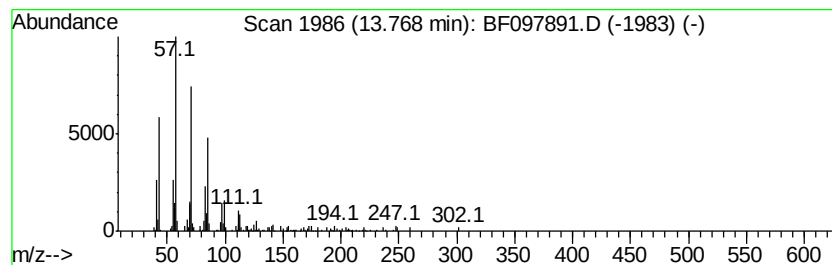
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tritetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.44 ng	94772	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tritetracontane	605	C43H88	007098-21-7	91
2		Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Heptadecane	240	C17H36	000629-78-7	72
5		Hexadecane	226	C16H34	000544-76-3	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
Data File : BF097891.D
Acq On : 19 Aug 2017 21:00
Operator : SJ/JU
Sample : I4845-01 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-81617

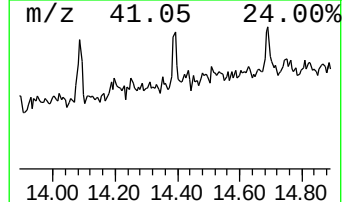
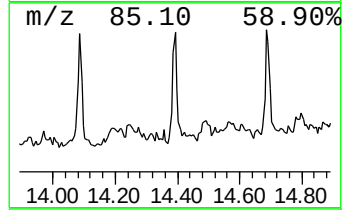
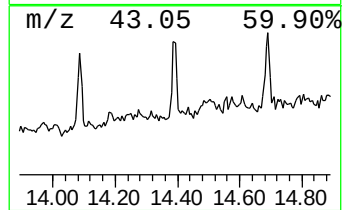
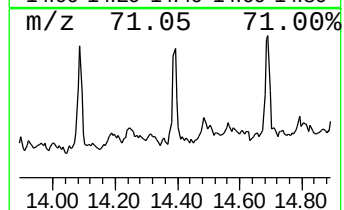
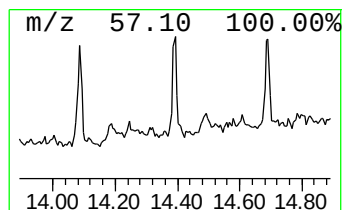
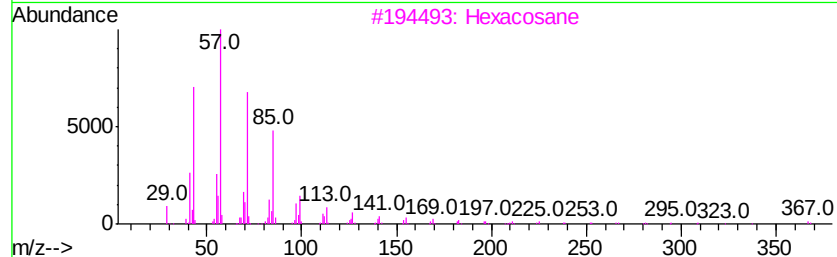
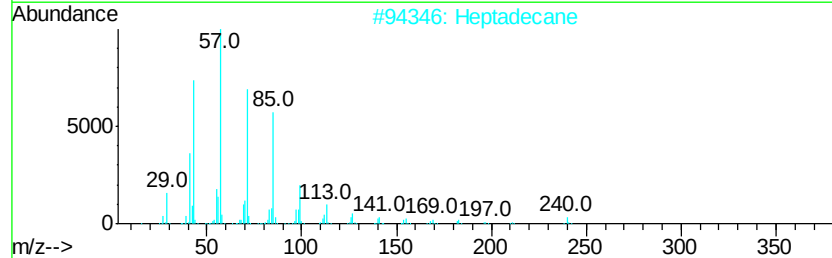
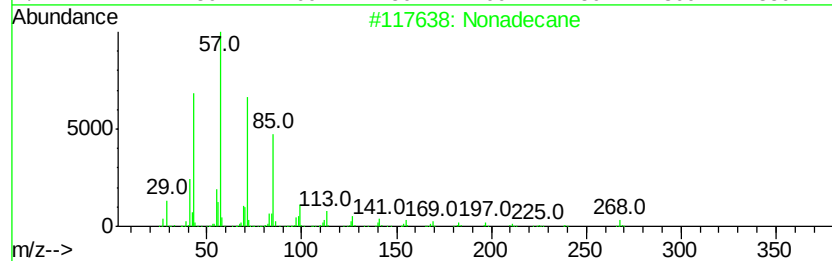
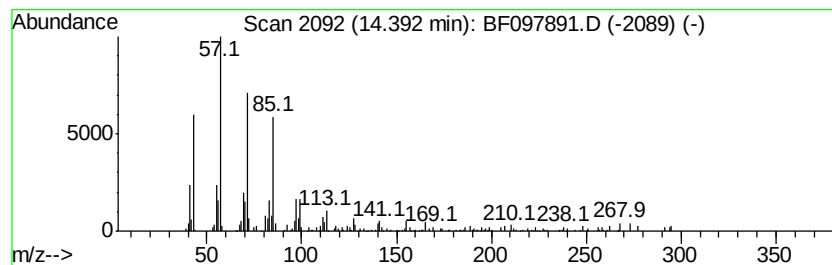
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.39	2.40 ng	93205	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	96
2	Heptadecane		240	C17H36	000629-78-7	93
3	Hexacosane		366	C26H54	000630-01-3	90
4	Heptacosane		380	C27H56	000593-49-7	90
5	Pentadecane		212	C15H32	000629-62-9	90



Data Path : Z:\HPCHEM1\BNA F\DATA\BF081917\
Data File : BF097891.D
Acq On : 19 Aug 2017 21:00
Operator : SJ/JU
Sample : I4845-01 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

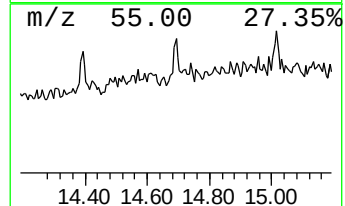
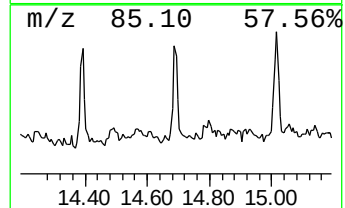
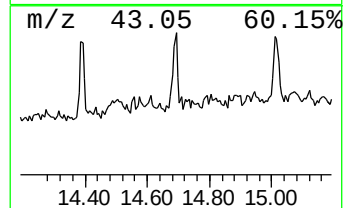
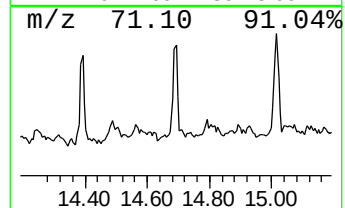
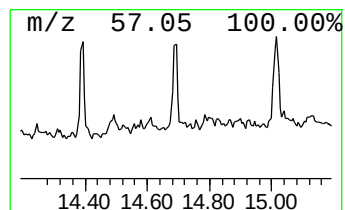
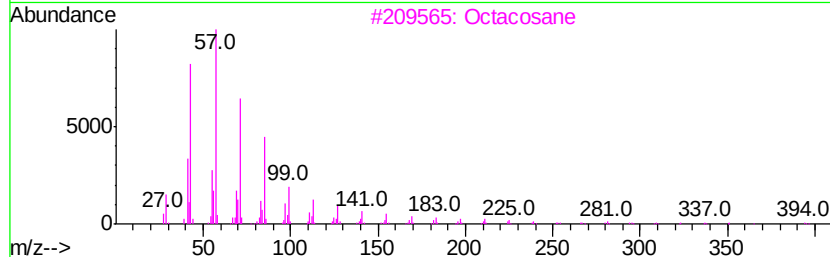
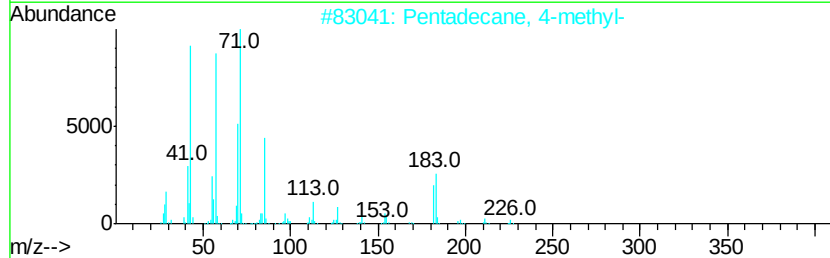
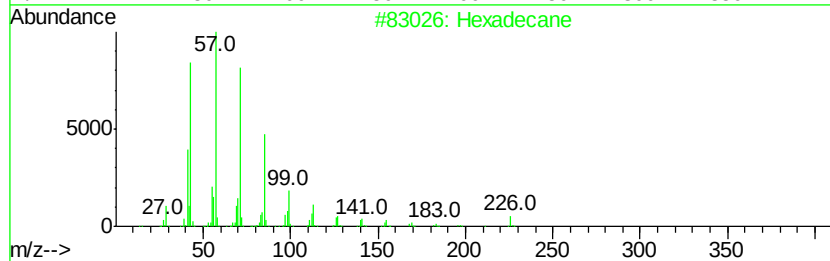
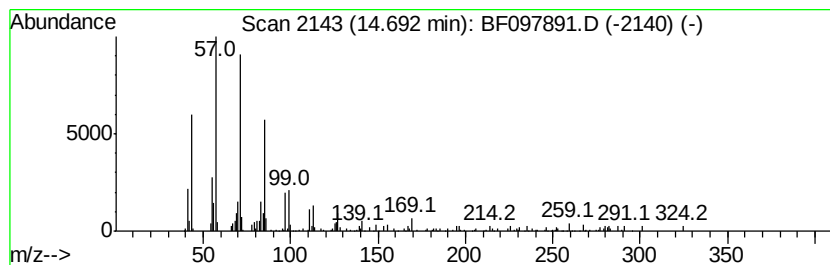
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.69	3.20 ng	84826	Perylene-d12		15.33		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Pentadecane, 4-methyl-	226	C16H34	002801-87-8	89
3			Octacosane	394	C28H58	000630-02-4	86
4			Docosane, 7-hexyl-	394	C28H58	055373-86-9	86
5			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	86



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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Sample : I4845-01 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

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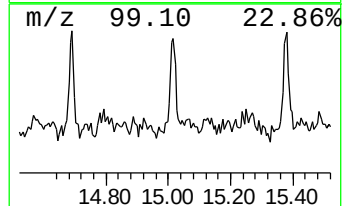
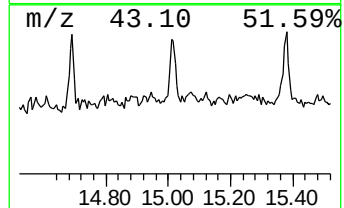
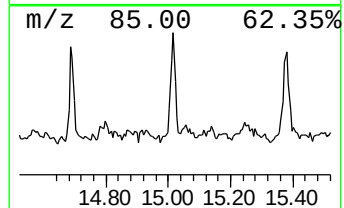
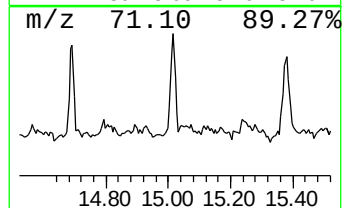
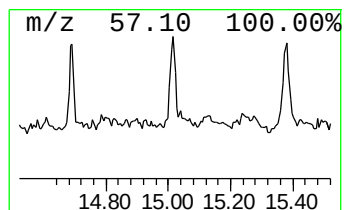
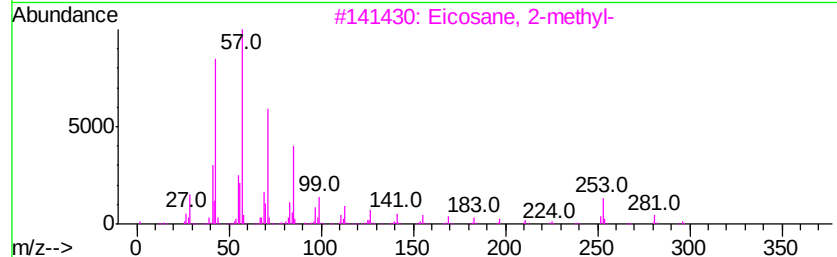
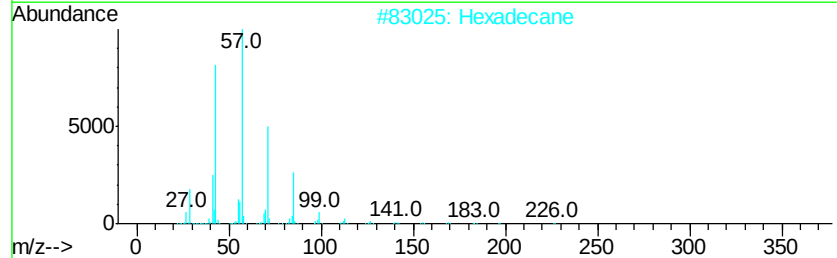
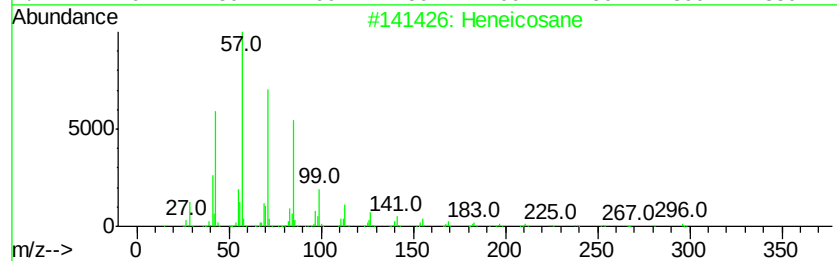
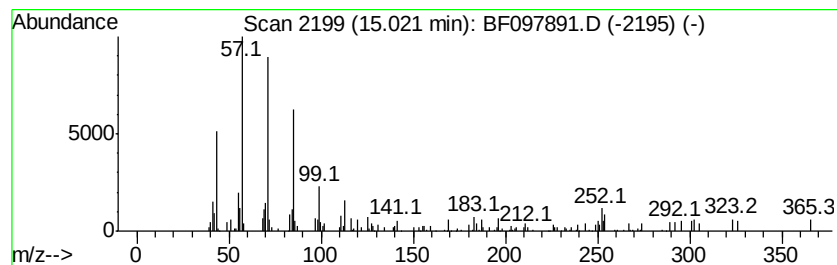
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.57 ng	94575	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	93
2	Hexadecane		226	C16H34	000544-76-3	93
3	Eicosane, 2-methyl-		296	C21H44	001560-84-5	91
4	10-Methylnonadecane		282	C20H42	056862-62-5	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081917\
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Acq On : 19 Aug 2017 21:00
Operator : SJ/JU
Sample : I4845-01 10X
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OK-03-81617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.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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Tridecane	10.70	3.0	ng	141213	4	11.27	937300	20.0
Hexadecanoic acid...	11.67	3.7	ng	173087	4	11.27	937300	20.0
9,12-Octadecadien...	12.36	14.9	ng	696975	4	11.27	937300	20.0
9-Octadecenoic ac...	12.38	7.3	ng	344185	4	11.27	937300	20.0
Tritetracontane	13.77	2.4	ng	94772	5	13.90	777488	20.0
Nonadecane	14.39	2.4	ng	93205	5	13.90	777488	20.0
Hexadecane	14.69	3.2	ng	84826	6	15.33	529545	20.0
Heneicosane	15.02	3.6	ng	94575	6	15.33	529545	20.0