

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
 Data File : BF103773.D
 Acq On : 19 Mar 2018 23:12
 Operator : JU/SJ
 Sample : J1972-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-1 COMP

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-BF031518.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.346	37	44	50	rVB	160129	224066	5.45%	0.564%
2	5.228	530	534	543	rVB	162066	218487	5.32%	0.550%
3	5.604	592	598	601	rBV	3724765	4076814	99.19%	10.259%
4	5.922	648	652	659	rVB	53588	49565	1.21%	0.125%
5	6.598	760	767	770	rBV	3483288	4109922	100.00%	10.343%
6	6.745	786	792	795	rBV	3954939	4097494	99.70%	10.311%
7	6.975	827	831	834	rVB	1023515	889322	21.64%	2.238%
8	7.134	853	858	861	rBV	3193041	3209314	78.09%	8.076%
9	7.539	920	927	930	rBV	2361439	2660347	64.73%	6.695%
10	7.598	933	937	946	rVB	39265	43998	1.07%	0.111%
11	8.251	1044	1048	1052	rBV	1288890	1157444	28.16%	2.913%
12	9.327	1225	1231	1234	rBV	4043926	3927352	95.56%	9.883%
13	9.716	1291	1297	1300	rBV	455302	345600	8.41%	0.870%
14	9.927	1329	1333	1336	rBV	106140	76834	1.87%	0.193%
15	10.016	1344	1348	1351	rBV	1191308	1125395	27.38%	2.832%
16	10.427	1416	1418	1421	rVB	131222	93583	2.28%	0.236%
17	10.651	1449	1456	1458	rBV2	37470	46362	1.13%	0.117%
18	10.804	1478	1482	1486	rBV	2206859	2113749	51.43%	5.319%
19	10.904	1496	1499	1509	rVB	107246	121570	2.96%	0.306%
20	11.351	1572	1575	1578	rBV	67520	57863	1.41%	0.146%
21	11.504	1597	1601	1604	rBV	1120144	984307	23.95%	2.477%
22	11.527	1604	1605	1610	rVV	297633	201367	4.90%	0.507%
23	11.580	1610	1614	1617	rVB	73799	61244	1.49%	0.154%
24	12.010	1683	1687	1689	rBV2	98528	96860	2.36%	0.244%
25	12.033	1689	1691	1697	rVB2	70174	64168	1.56%	0.161%
26	12.121	1702	1706	1708	rBV2	57795	60568	1.47%	0.152%
27	12.721	1804	1808	1812	rBV	511365	414621	10.09%	1.043%
28	12.951	1841	1847	1853	rBV	440405	496055	12.07%	1.248%
29	13.092	1867	1871	1875	rBV	2742493	2688299	65.41%	6.765%
30	13.168	1880	1884	1888	rBV3	33411	53464	1.30%	0.135%
31	13.280	1900	1903	1906	rVB	70832	67558	1.64%	0.170%
32	13.386	1917	1921	1924	rBV	94752	95186	2.32%	0.240%
33	13.480	1934	1937	1939	rBV2	69537	58782	1.43%	0.148%
34	13.510	1939	1942	1945	rVV	58584	51532	1.25%	0.130%

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Integration Parameters: rteint.p
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 Min Area: 3 % of largest Peak
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.792	1987	1990	1995	rVB	72768	78151	1.90%	0.197%
36	13.851	1995	2000	2003	rBV	77143	74054	1.80%	0.186%
37	13.892	2003	2007	2008	rBV	89639	96215	2.34%	0.242%
38	13.910	2008	2010	2012	rVB2	79496	64276	1.56%	0.162%
39	13.974	2016	2021	2024	rBV3	191658	245342	5.97%	0.617%
40	14.121	2043	2046	2047	rBV2	45060	45413	1.10%	0.114%
41	14.157	2047	2052	2055	rVV2	1085077	1251223	30.44%	3.149%
42	14.180	2055	2056	2063	rVB	331006	266727	6.49%	0.671%
43	14.239	2063	2066	2068	rBV2	99969	95894	2.33%	0.241%
44	14.392	2087	2092	2094	rBV3	52431	85282	2.08%	0.215%
45	14.509	2109	2112	2114	rBV2	51482	50502	1.23%	0.127%
46	14.551	2114	2119	2122	rVV2	165081	250200	6.09%	0.630%
47	14.580	2122	2124	2127	rVV	109780	120567	2.93%	0.303%
48	14.615	2127	2130	2133	rVV2	88209	123535	3.01%	0.311%
49	14.674	2137	2140	2143	rVV2	80498	107849	2.62%	0.271%
50	14.698	2143	2144	2149	rVV3	60496	61436	1.49%	0.155%
51	14.745	2149	2152	2156	rVB4	34350	45589	1.11%	0.115%
52	14.898	2174	2178	2180	rBV	96370	135914	3.31%	0.342%
53	14.951	2185	2187	2190	rVV	107498	143311	3.49%	0.361%
54	14.992	2191	2194	2196	rVV	95478	120514	2.93%	0.303%
55	15.015	2196	2198	2204	rVB2	59149	78214	1.90%	0.197%
56	15.239	2231	2236	2239	rBV	222450	359910	8.76%	0.906%
57	15.351	2253	2255	2259	rVB	44629	41501	1.01%	0.104%
58	15.562	2287	2291	2297	rBV	170606	217689	5.30%	0.548%
59	15.627	2298	2302	2308	rVB	220070	302083	7.35%	0.760%
60	15.698	2309	2314	2317	rBV	521010	673193	16.38%	1.694%
61	15.727	2317	2319	2327	rVB2	70081	92526	2.25%	0.233%
62	16.168	2391	2394	2398	rVB2	54932	72651	1.77%	0.183%
63	16.715	2483	2487	2489	rBV3	26533	45076	1.10%	0.113%
64	17.262	2575	2580	2588	rVB2	100066	203395	4.95%	0.512%
65	17.745	2657	2662	2671	rVB2	72283	150144	3.65%	0.378%

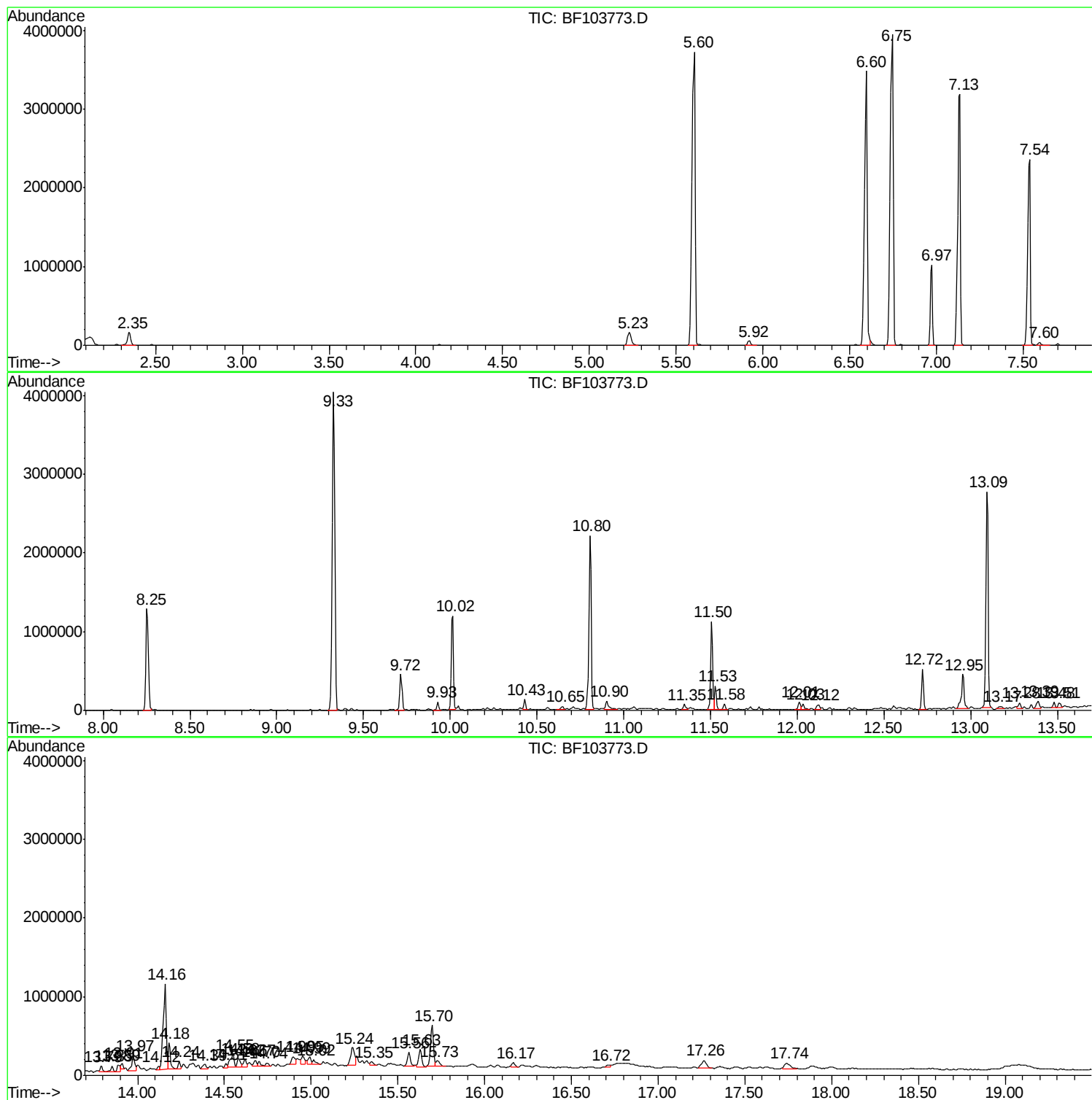
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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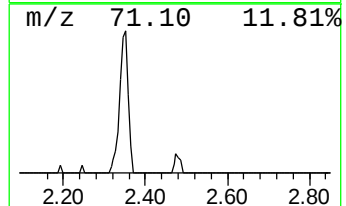
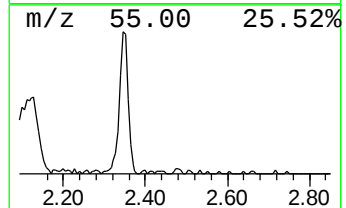
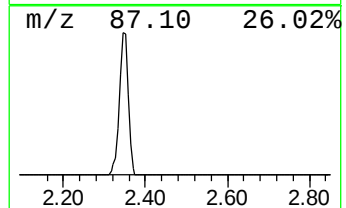
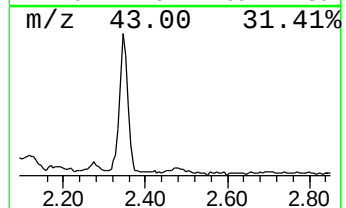
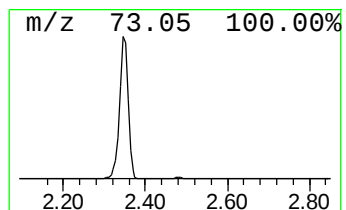
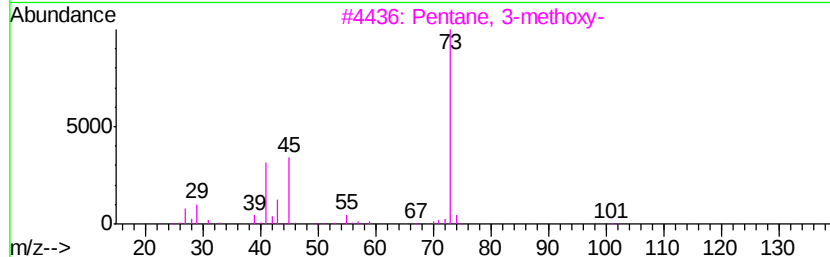
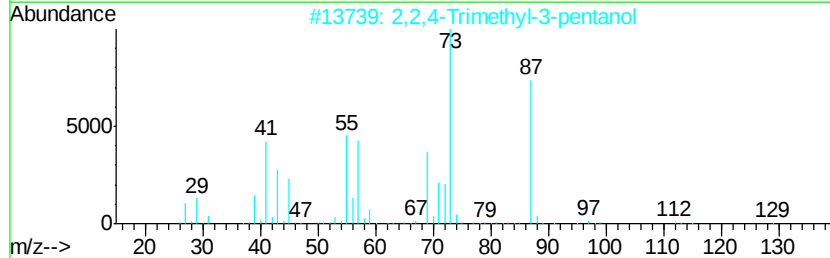
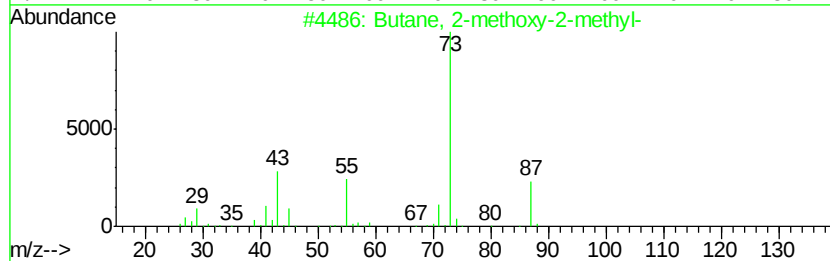
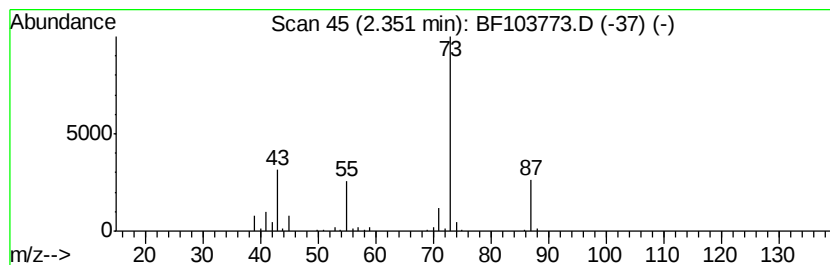
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.35	5.04 ng	224066	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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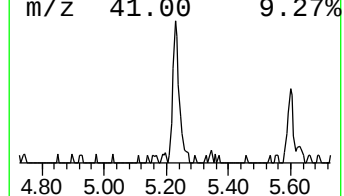
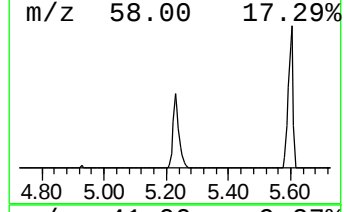
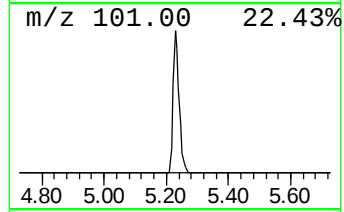
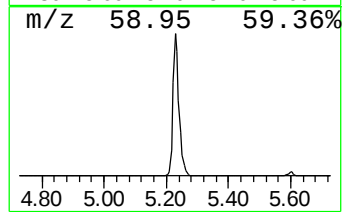
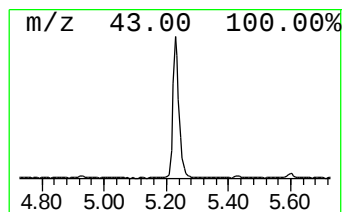
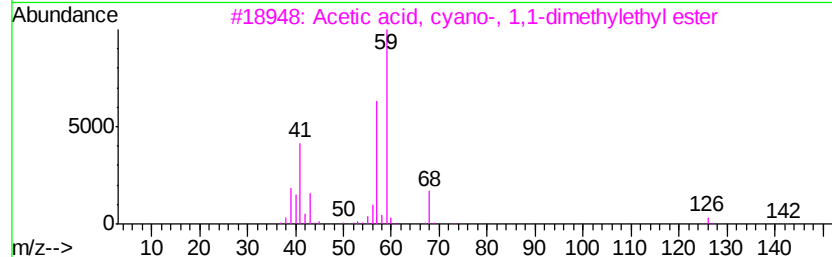
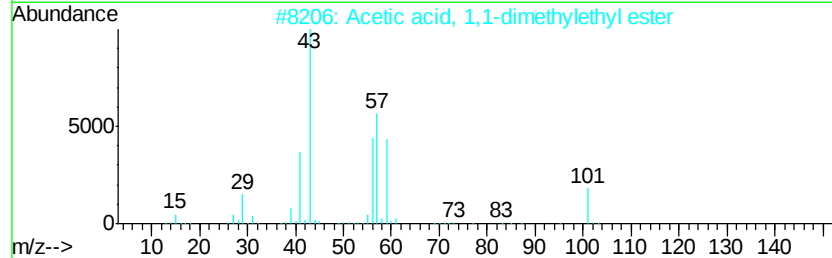
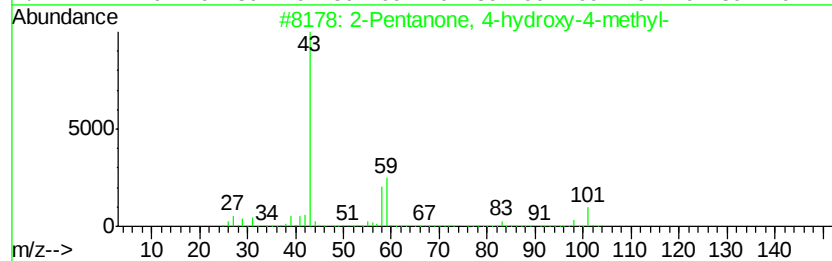
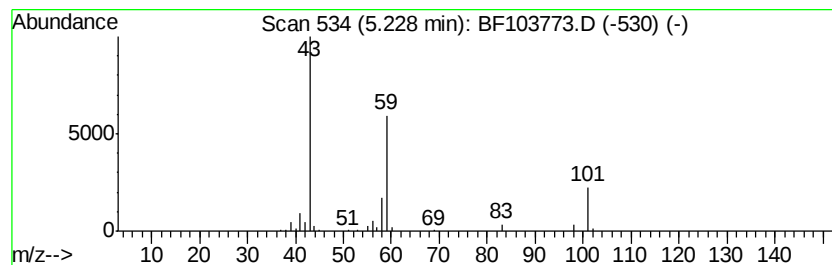
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	4.91 ng	218487	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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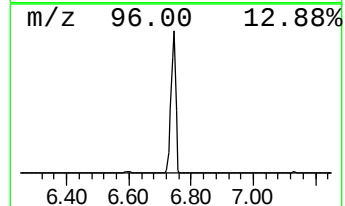
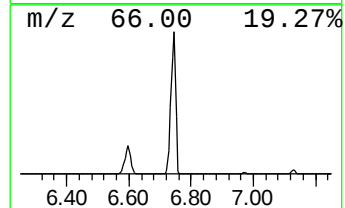
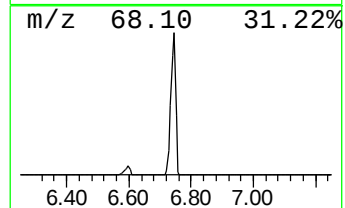
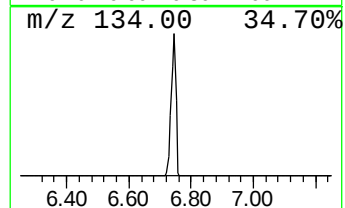
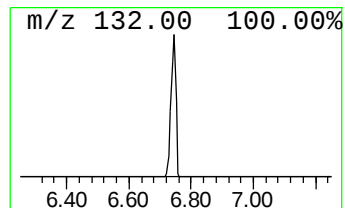
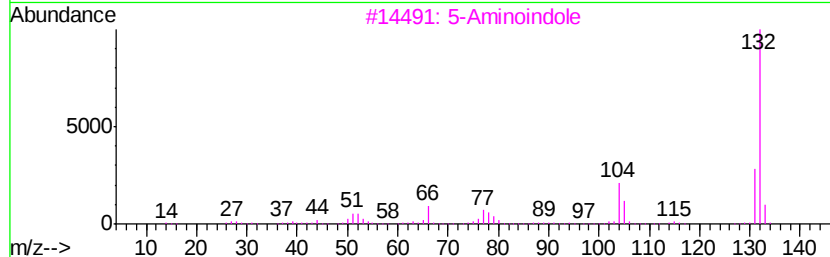
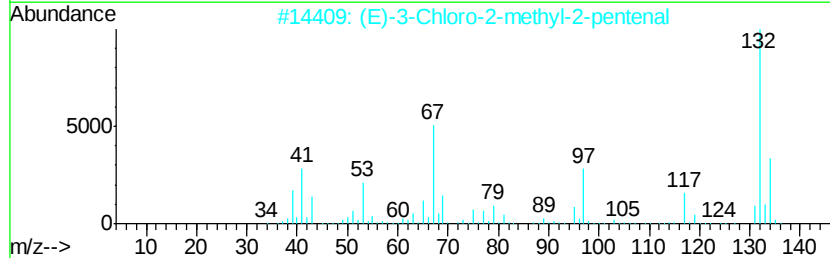
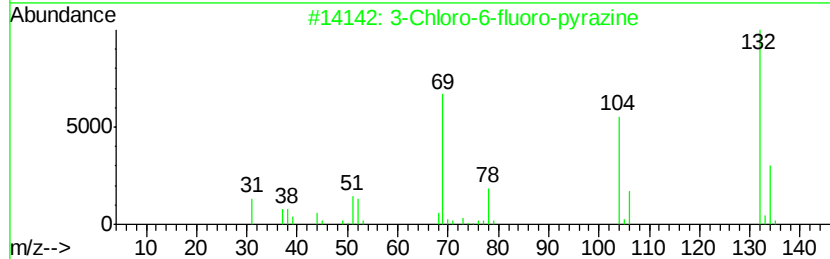
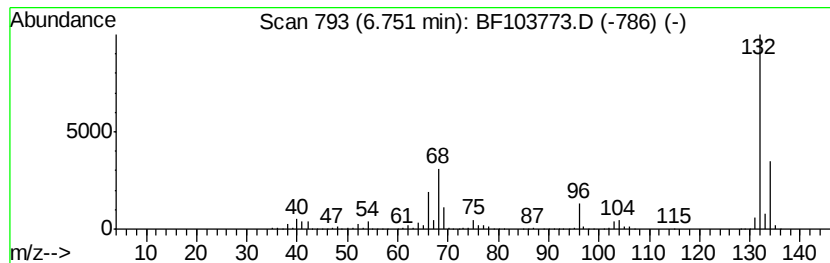
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	92.15 ng	4097490	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
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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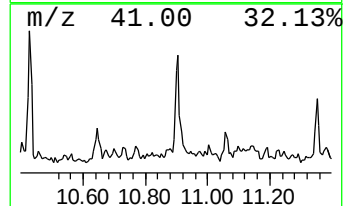
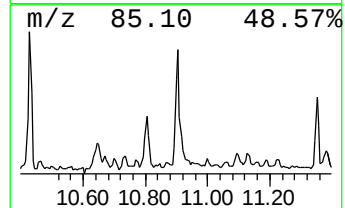
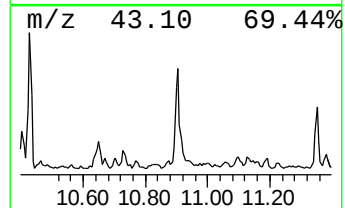
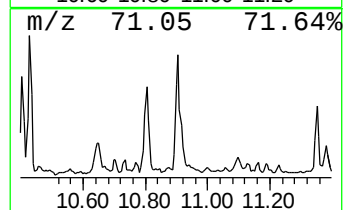
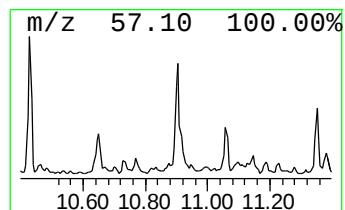
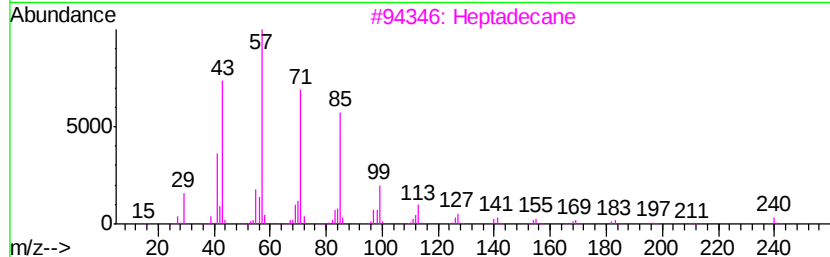
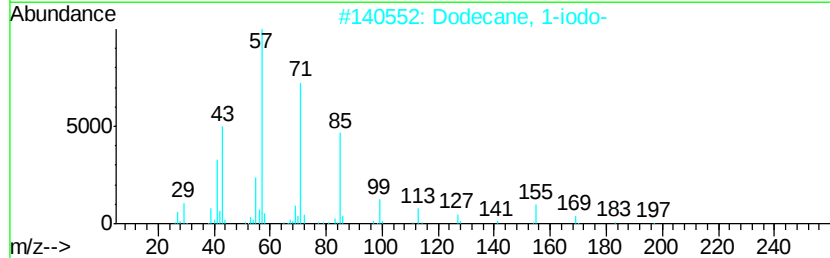
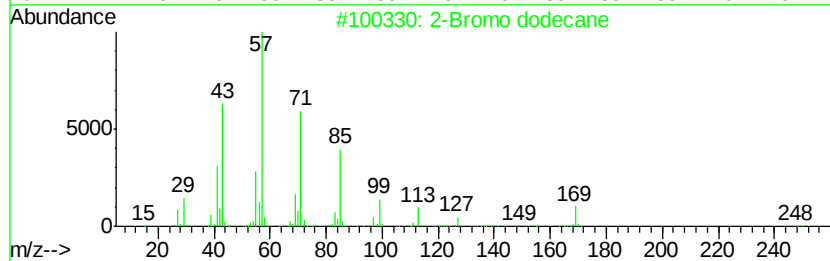
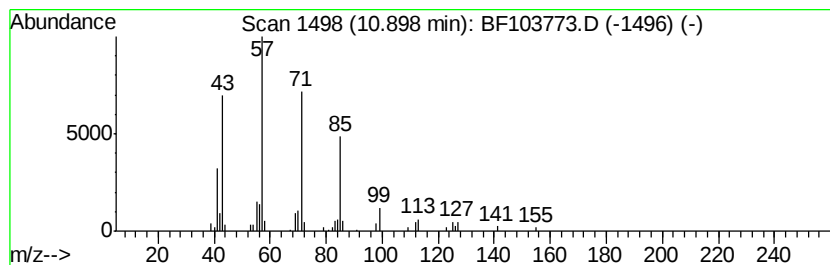
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Bromo dodecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.47 ng	121570	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane		248	C12H25Br	013187-99-0	90
2	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	90
3	Heptadecane		240	C17H36	000629-78-7	90
4	Eicosane		282	C20H42	000112-95-8	90
5	Hexadecane		226	C16H34	000544-76-3	90



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S-1 COMP

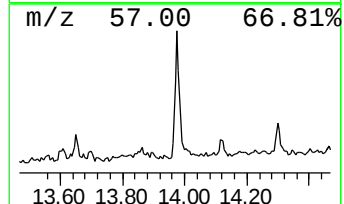
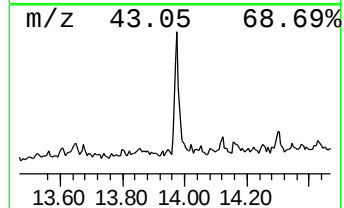
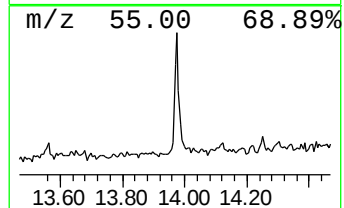
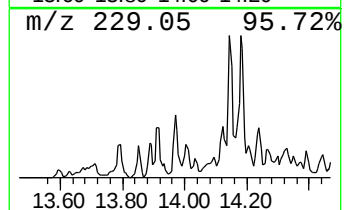
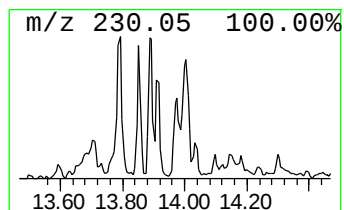
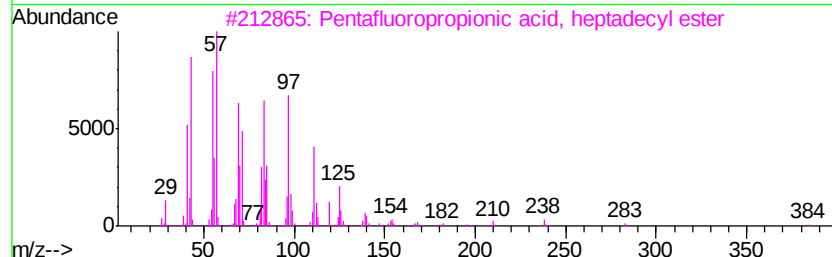
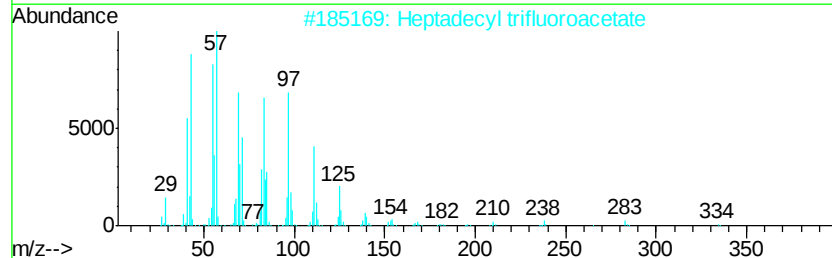
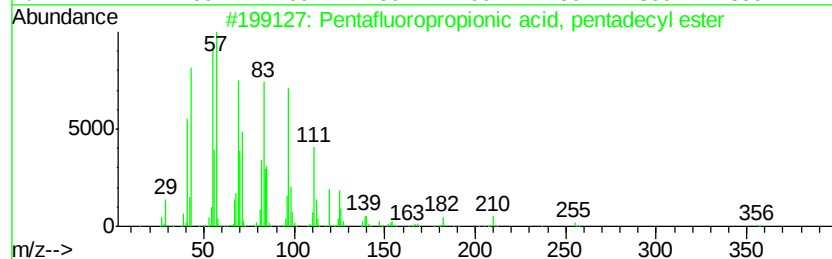
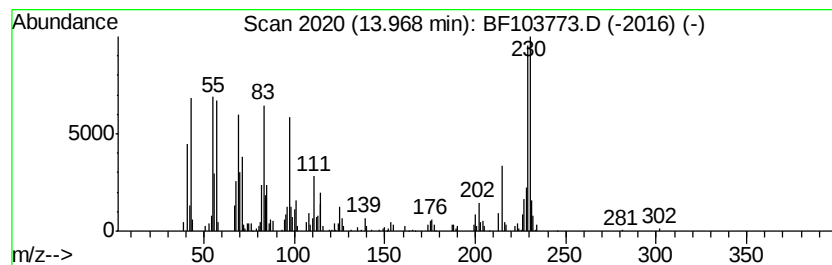
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.92 ng	245342	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	80
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	78
5		n-Heptadecanol-1	256	C17H36O	001454-85-9	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103773.D
Acq On : 19 Mar 2018 23:12
Operator : JU/SJ
Sample : J1972-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1 COMP

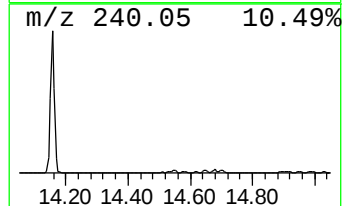
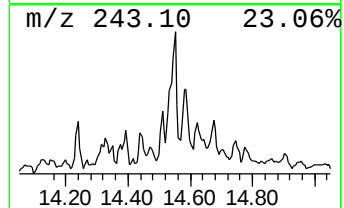
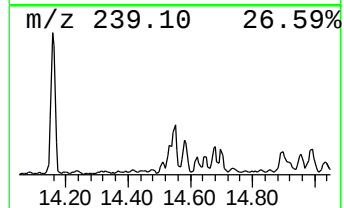
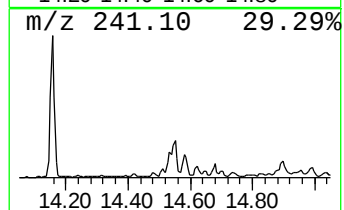
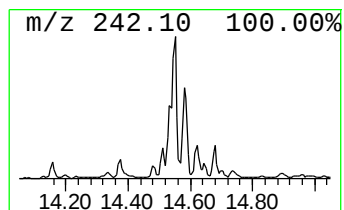
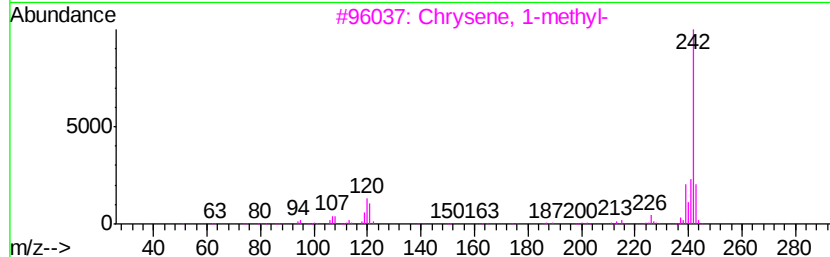
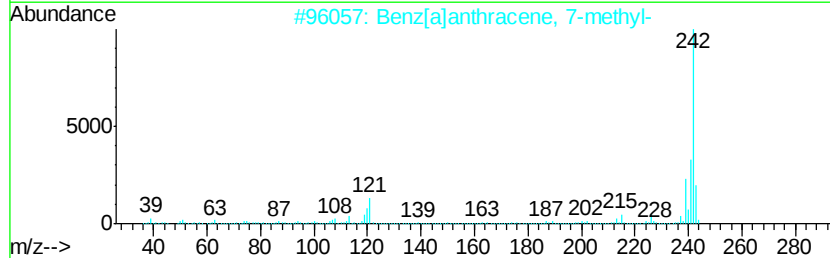
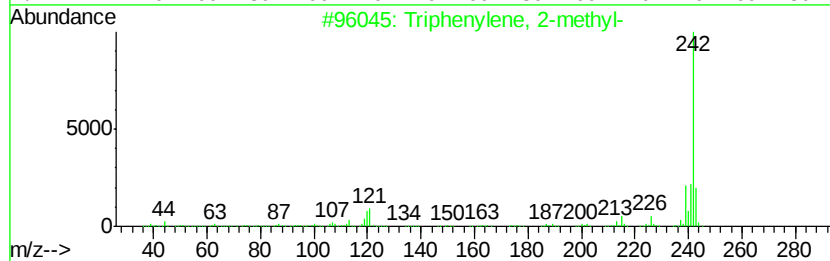
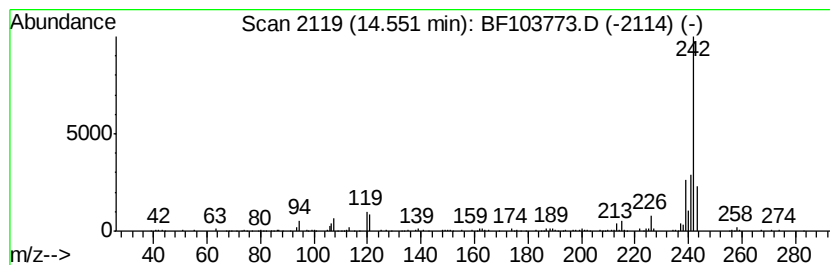
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.55	4.00 ng	250200	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylene, 2-methyl-	242	C19H14	001705-84-6	94
2	Benz[a]anthracene, 7-methyl-	242	C19H14	002541-69-7	93
3	Chrysene, 1-methyl-	242	C19H14	003351-28-8	91
4	Benz[a]anthracene, 8-methyl-	242	C19H14	002381-31-9	89
5	Chrysene, 6-methyl-	242	C19H14	001705-85-7	81



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
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Acq On : 19 Mar 2018 23:12
Operator : JU/SJ
Sample : J1972-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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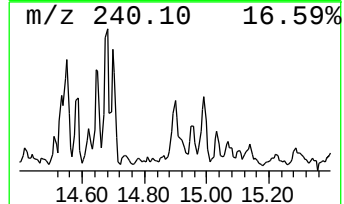
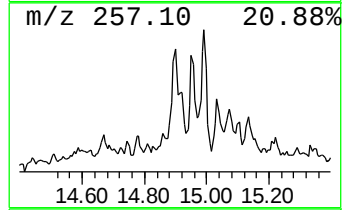
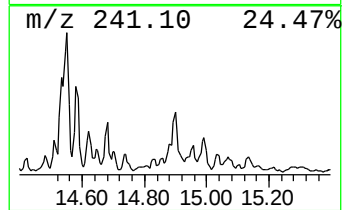
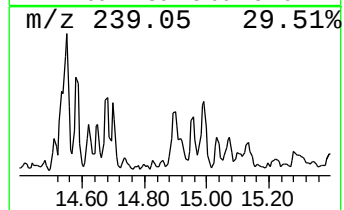
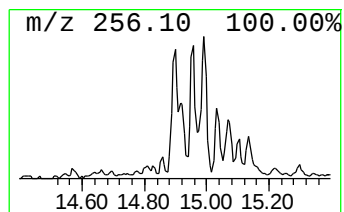
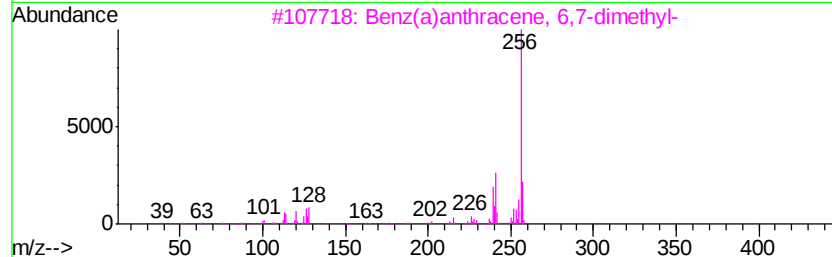
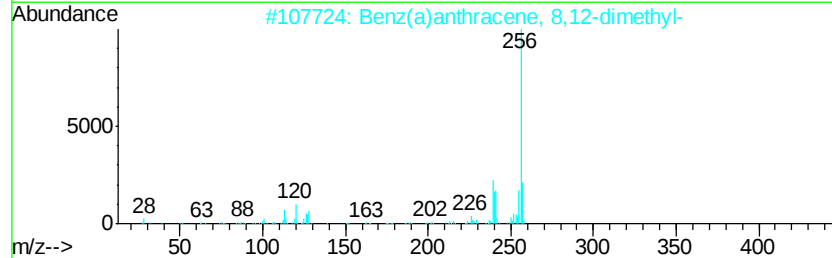
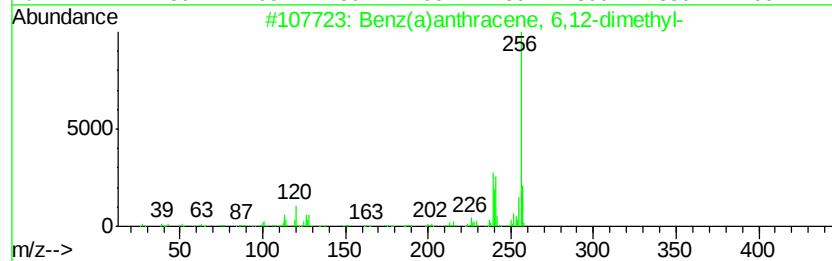
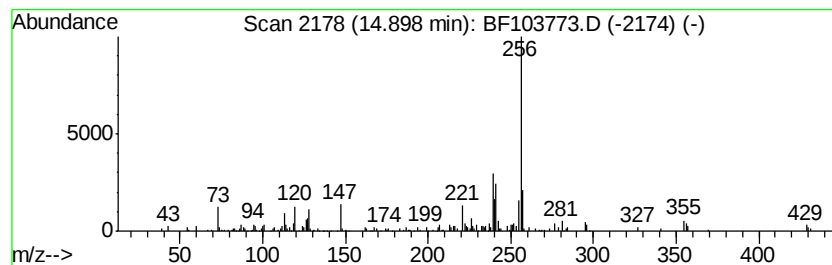
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benz(a)anthracene, 6,12-dim... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	2.17 ng	135914	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benz(a)anthracene, 6,12-dimethyl-	256	C20H16	000568-81-0	94
2		Benz(a)anthracene, 8,12-dimethyl-	256	C20H16	020627-31-0	93
3		Benz(a)anthracene, 6,7-dimethyl-	256	C20H16	020627-28-5	93
4		4,12-Dimethylbenz[<i>a</i>]anthracene	256	C20H16	035187-19-0	93
5		Benz(a)anthracene, 6,8-dimethyl-	256	C20H16	000317-64-6	90



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103773.D
Acq On : 19 Mar 2018 23:12
Operator : JU/SJ
Sample : J1972-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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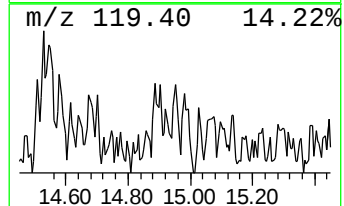
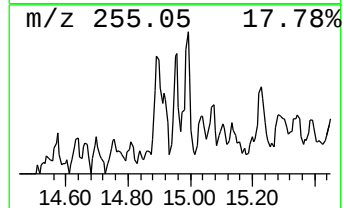
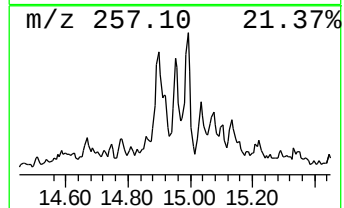
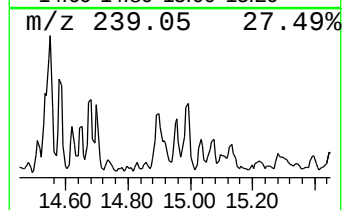
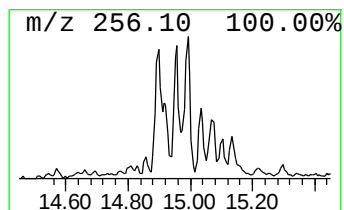
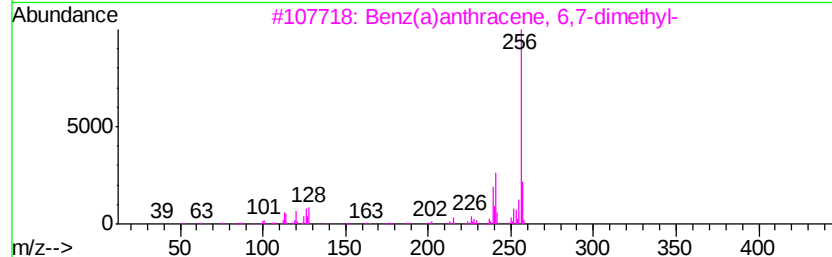
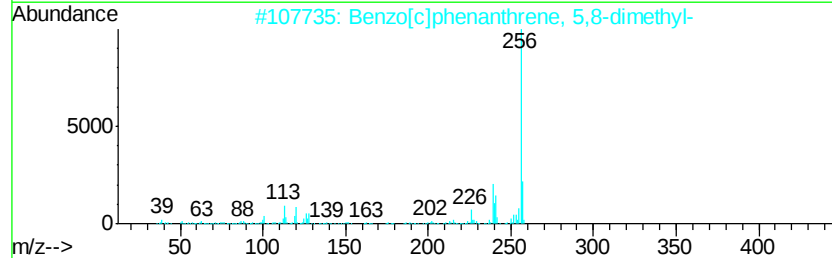
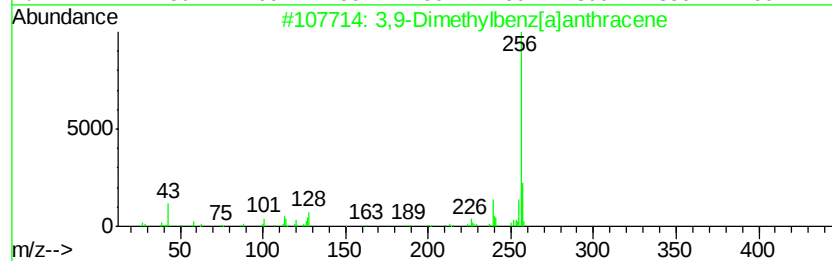
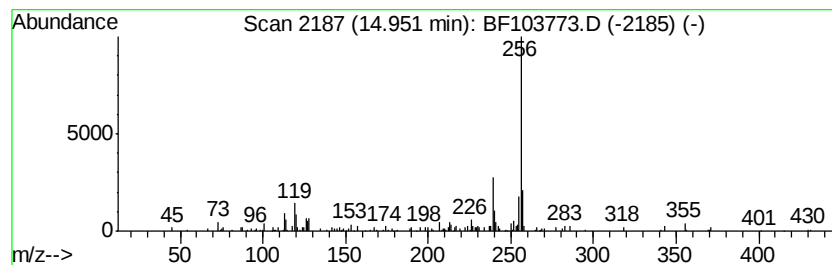
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3,9-Dimethylbenz[a]anthracene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	4.26 ng	143311	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,9-Dimethylbenz[a]anthracene	256	C20H16	000316-51-8	98
2		Benzo[c]phenanthrene, 5,8-dimethyl-	256	C20H16	054986-63-9	93
3		Benz(a)anthracene, 6,7-dimethyl-	256	C20H16	020627-28-5	93
4		5,12-Dimethylbenz[a]anthracene	256	C20H16	021297-22-3	91
5		Benz(a)anthracene, 7,8-dimethyl-	256	C20H16	000604-81-9	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103773.D
Acq On : 19 Mar 2018 23:12
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Instrument :
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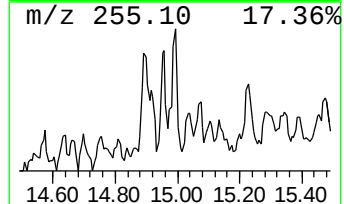
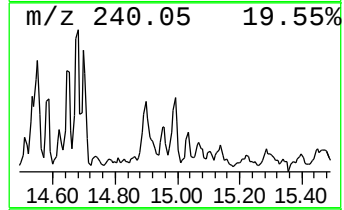
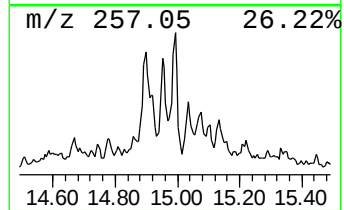
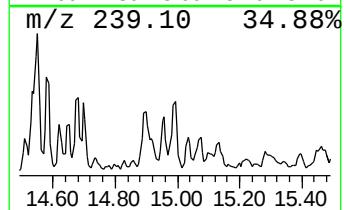
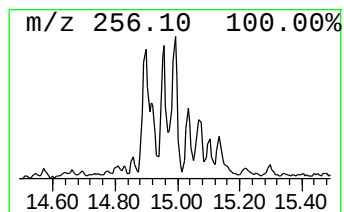
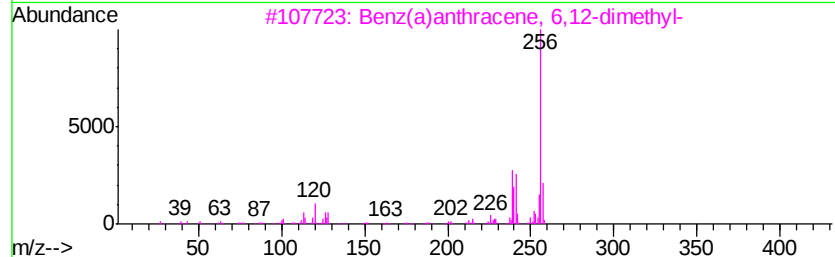
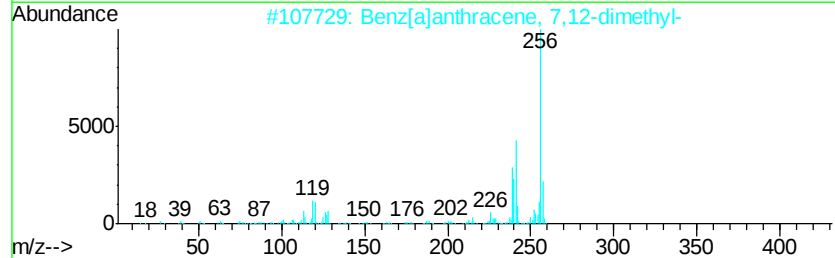
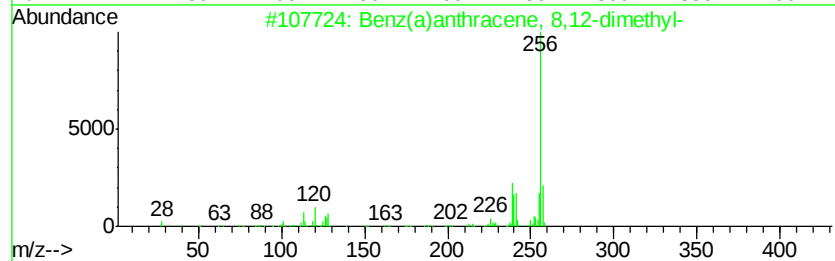
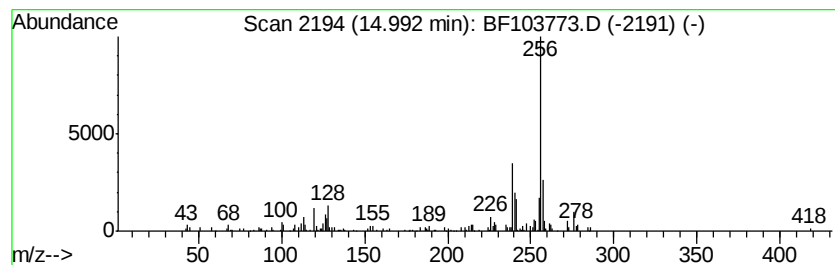
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benz(a)anthracene, 8,12-dim... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	3.58 ng	120514	Perylene-d12	15.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz(a)anthracene, 8,12-dimethyl-	256	C20H16	020627-31-0	94
2			Benz[a]anthracene, 7,12-dimethyl-	256	C20H16	000057-97-6	91
3			Benz(a)anthracene, 6,12-dimethyl-	256	C20H16	000568-81-0	87
4			5,12-Dimethylbenz[a]anthracene	256	C20H16	021297-22-3	87
5			Chrysene, 5-ethyl-	256	C20H16	054986-62-8	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
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Acq On : 19 Mar 2018 23:12
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Sample : J1972-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

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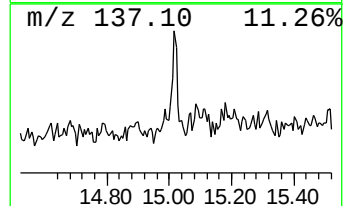
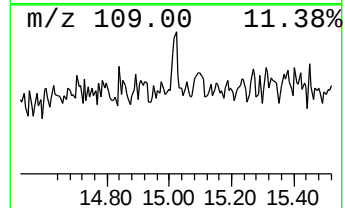
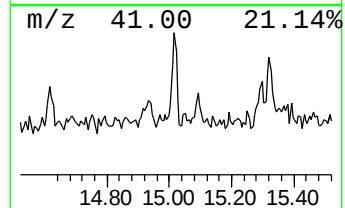
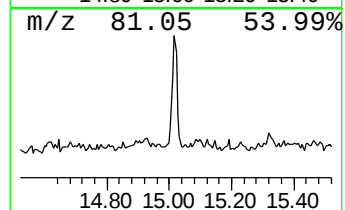
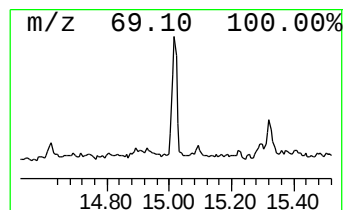
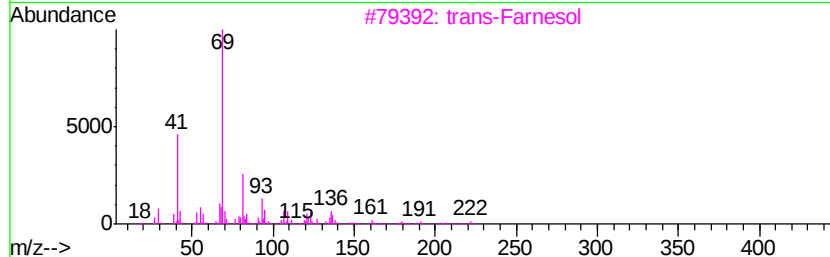
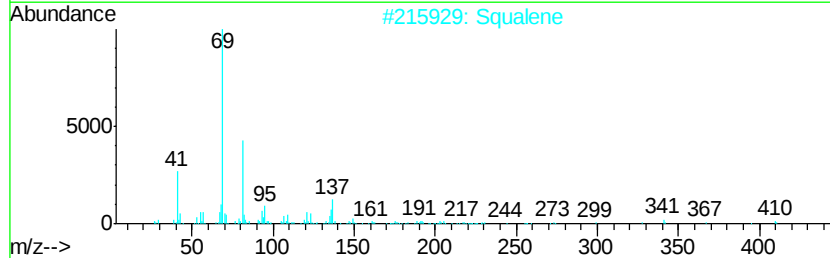
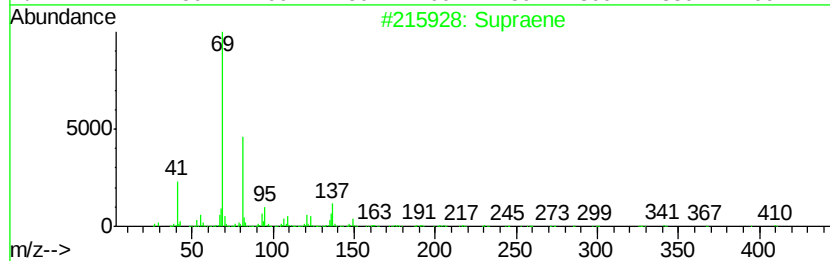
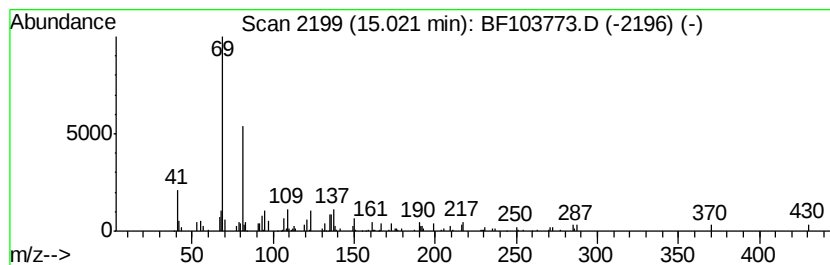
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Supraene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.32 ng	78214	Perylene-d12	15.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	80
2			Squalene	410	C30H50	000111-02-4	80
3			trans-Farnesol	222	C15H26O	000106-28-5	64
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5			3,7,11-Tridecatrienoic acid, 4,8...	264	C17H28O2	036237-69-1	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
Data File : BF103773.D
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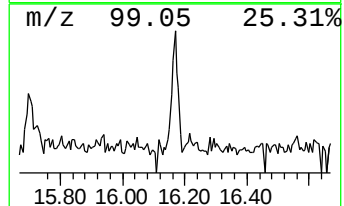
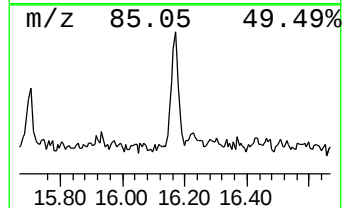
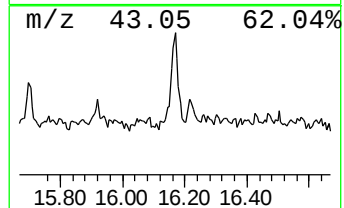
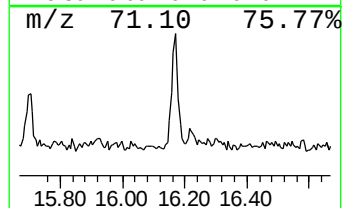
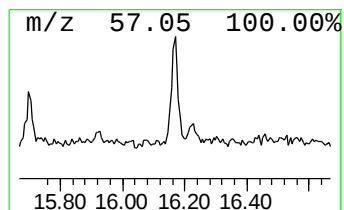
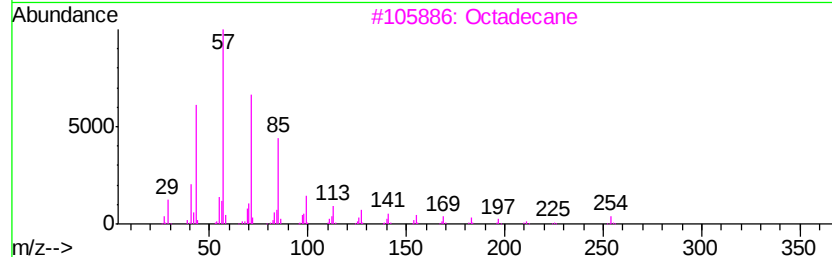
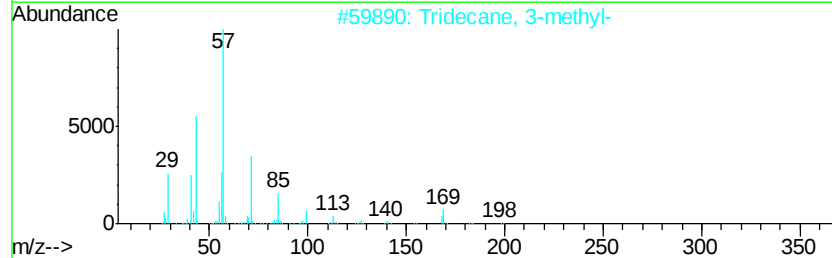
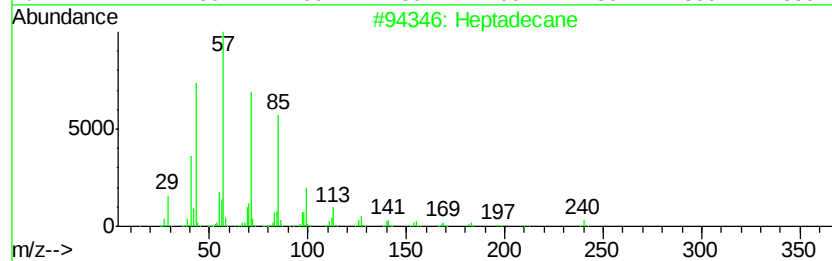
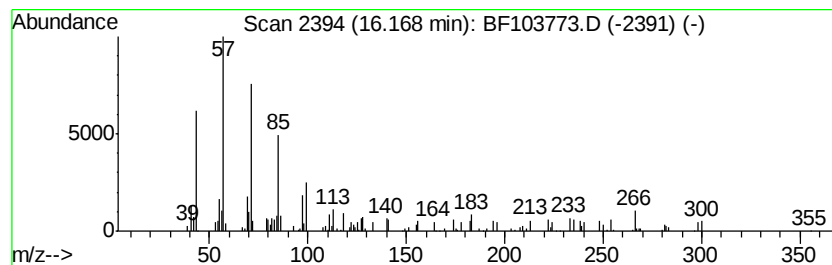
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Heptadecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	2.16 ng	72651	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	90
2		Tridecane, 3-methyl-	198	C14H30	006418-41-3	64
3		Octadecane	254	C18H38	000593-45-3	64
4		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	64
5		Nonadecane	268	C19H40	000629-92-5	62



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103773.D
Acq On : 19 Mar 2018 23:12
Operator : JU/SJ
Sample : J1972-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
S-1 COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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
Butane, 2-methoxy...	2.35	5.0	ng	224066	1	6.97	889322	20.0
2-Pentanone, 4-hy...	5.23	4.9	ng	218487	1	6.97	889322	20.0
unknown6.75	6.75	92.2	ng	4097490	1	6.97	889322	20.0
2-Bromo dodecane	10.90	2.5	ng	121570	4	11.50	984307	20.0
Pentafluoropropio...	13.97	3.9	ng	245342	5	14.16	1251220	20.0
Triphenylene, 2-m...	14.55	4.0	ng	250200	5	14.16	1251220	20.0
Benz(a)anthracene...	14.90	2.2	ng	135914	5	14.16	1251220	20.0
3,9-Dimethylbenz[...	14.95	4.3	ng	143311	6	15.70	673193	20.0
Benz(a)anthracene...	14.99	3.6	ng	120514	6	15.70	673193	20.0
Supraene	15.02	2.3	ng	78214	6	15.70	673193	20.0
Heptadecane	16.17	2.2	ng	72651	6	15.70	673193	20.0