

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031918\
 Data File : BF103766.D
 Acq On : 19 Mar 2018 20:03
 Operator : JU/SJ
 Sample : J1971-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ES-6-SA-2-EW@3

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	2.334	35	42	47	rVB	170030	241410	5.27%	0.572%
2	5.228	530	534	544	rVB	192393	274213	5.99%	0.650%
3	5.604	592	598	601	rBV	3975605	4475940	97.74%	10.608%
4	5.922	648	652	659	rVB	77588	72387	1.58%	0.172%
5	6.598	761	767	771	rBV	3540927	4579411	100.00%	10.853%
6	6.745	787	792	795	rBV	4158928	4498301	98.23%	10.661%
7	6.975	827	831	834	rVB	1177571	947288	20.69%	2.245%
8	7.133	853	858	861	rVB	3596933	3331896	72.76%	7.897%
9	7.539	921	927	930	rBV	2748717	2904875	63.43%	6.885%
10	7.598	933	937	944	rVB	52000	49342	1.08%	0.117%
11	8.257	1045	1049	1052	rBV	1444385	1267379	27.68%	3.004%
12	9.333	1225	1232	1235	rBV	4124025	4258062	92.98%	10.092%
13	9.427	1246	1248	1252	rVB	86081	77818	1.70%	0.184%
14	9.716	1292	1297	1300	rBV	413183	335960	7.34%	0.796%
15	9.927	1330	1333	1337	rVB	145058	107075	2.34%	0.254%
16	10.016	1344	1348	1351	rBV	1560722	1356578	29.62%	3.215%
17	10.427	1416	1418	1421	rVB	174466	135467	2.96%	0.321%
18	10.651	1450	1456	1458	rBV	50874	64676	1.41%	0.153%
19	10.810	1478	1483	1486	rBV	2749803	2766099	60.40%	6.556%
20	10.904	1496	1499	1508	rVB	148810	163765	3.58%	0.388%
21	11.057	1521	1525	1529	rVB	51239	48459	1.06%	0.115%
22	11.351	1572	1575	1577	rBV	86870	66779	1.46%	0.158%
23	11.380	1577	1580	1586	rVB2	44827	54204	1.18%	0.128%
24	11.504	1597	1601	1604	rBV	1349405	1278491	27.92%	3.030%
25	11.527	1604	1605	1610	rVB2	146435	122712	2.68%	0.291%
26	11.668	1625	1629	1633	rVB2	53571	50816	1.11%	0.120%
27	12.015	1681	1688	1694	rBV	358289	393402	8.59%	0.932%
28	12.327	1739	1741	1748	rVB2	33366	51498	1.12%	0.122%
29	12.721	1803	1808	1812	rBV	331896	318461	6.95%	0.755%
30	12.804	1819	1822	1828	rBV2	65916	74200	1.62%	0.176%
31	12.957	1841	1848	1850	rBV	236081	261441	5.71%	0.620%
32	13.098	1866	1872	1875	rBV	3559366	3642720	79.55%	8.633%
33	13.974	2017	2021	2026	rBV3	625103	593604	12.96%	1.407%
34	14.157	2047	2052	2055	rBV	1086623	1059982	23.15%	2.512%

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

35	14.180	2055	2056	2064	rVB	137655	123314	2.69%	0.292%
36	14.915	2176	2181	2190	rVB2	685749	926664	20.24%	2.196%
37	15.233	2232	2235	2238	rBV	134208	178059	3.89%	0.422%
38	15.562	2288	2291	2296	rVB	90462	120826	2.64%	0.286%
39	15.621	2299	2301	2309	rVB	97124	126056	2.75%	0.299%
40	15.698	2309	2314	2318	rBV	616846	794355	17.35%	1.883%

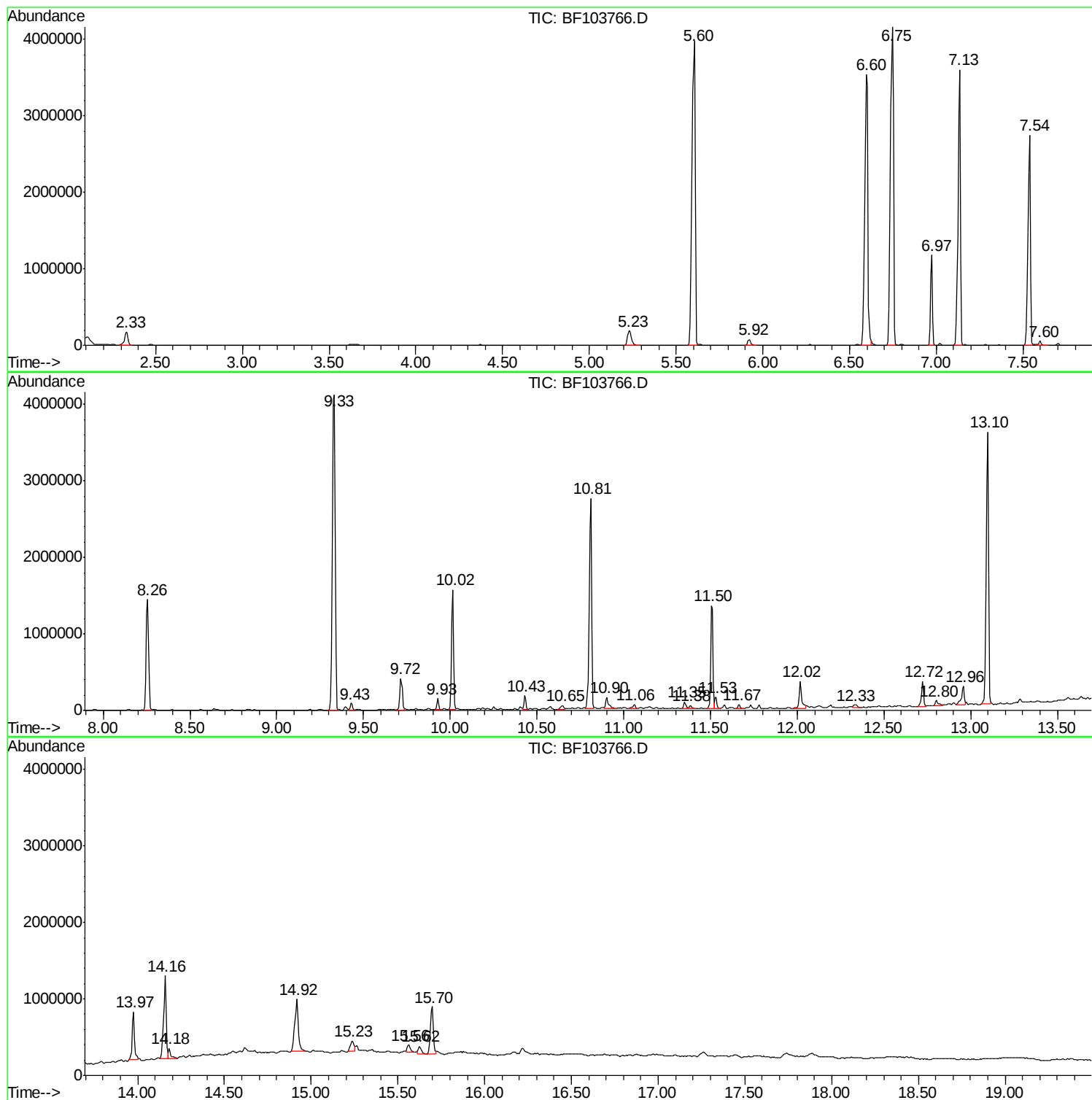
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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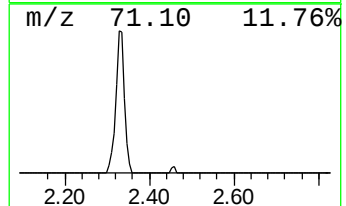
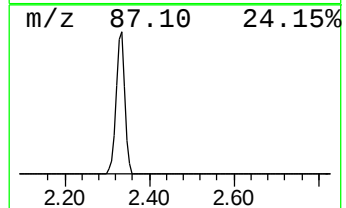
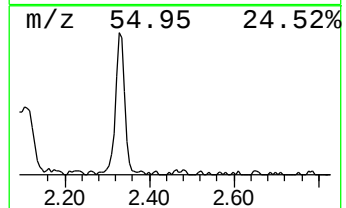
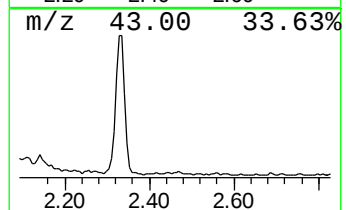
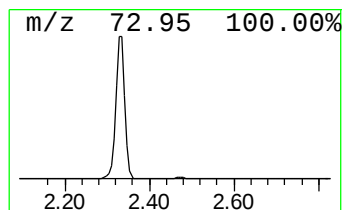
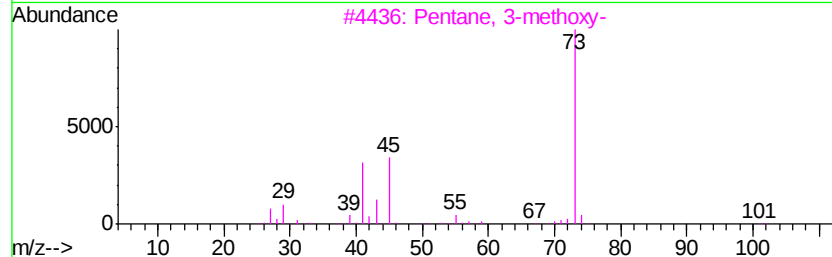
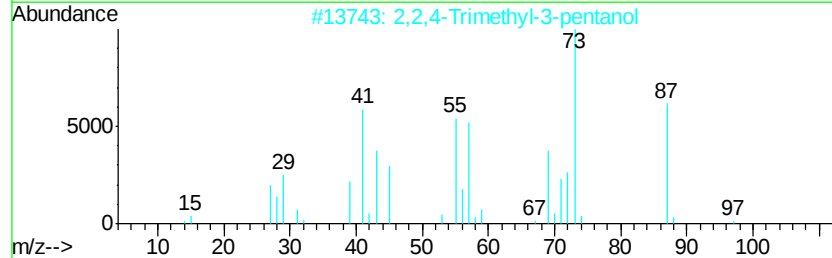
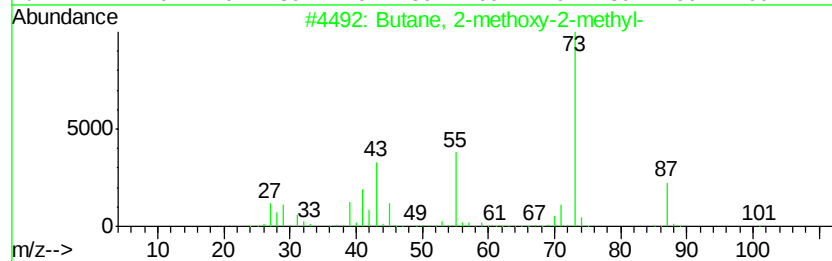
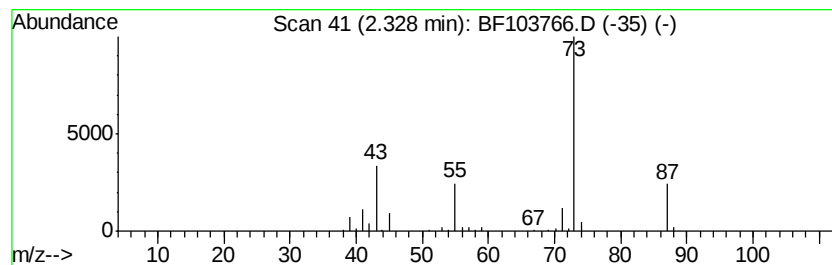
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	5.10 ng	241410	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10



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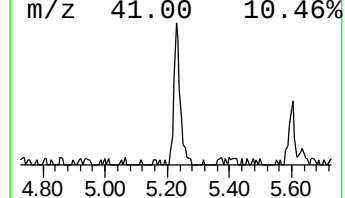
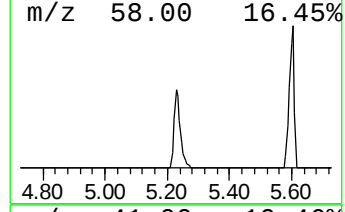
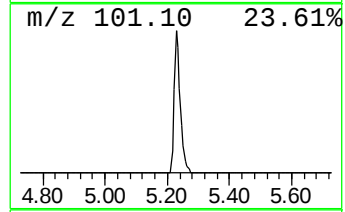
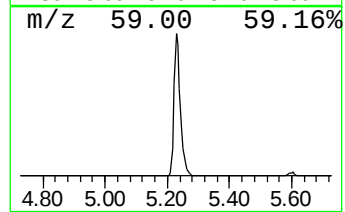
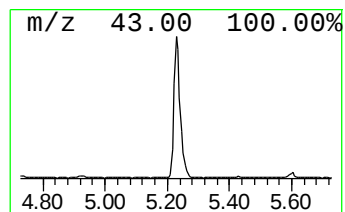
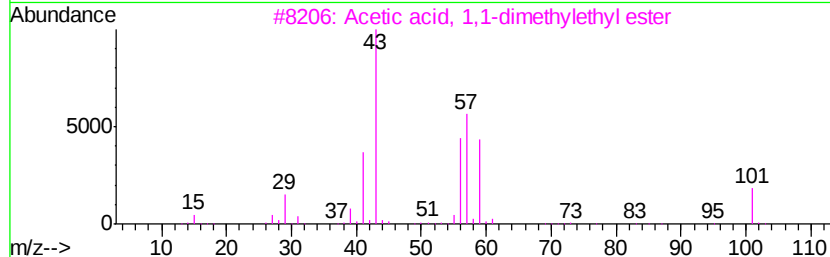
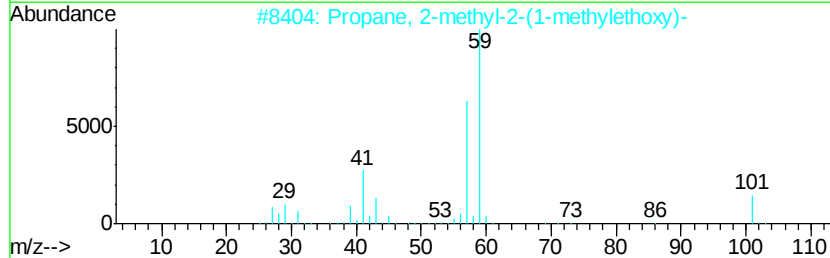
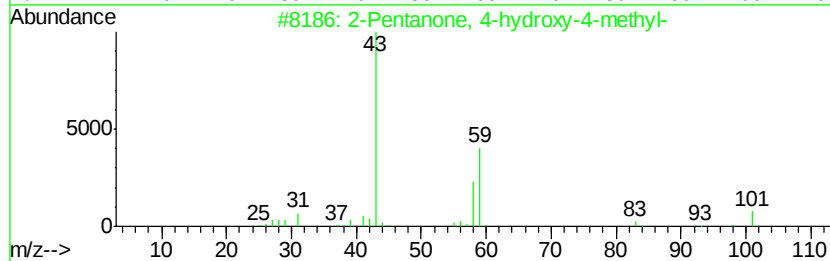
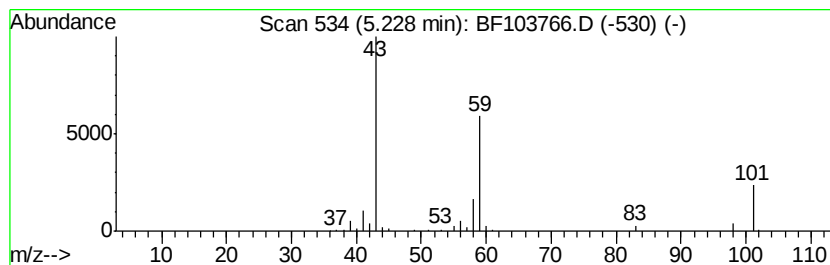
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	5.79 ng	274213	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	56
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	50
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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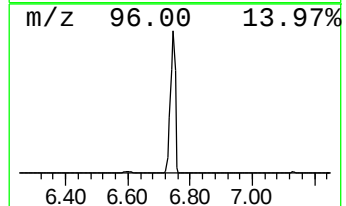
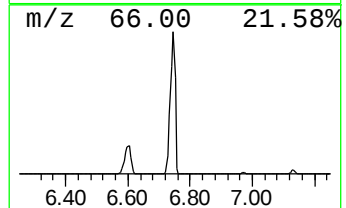
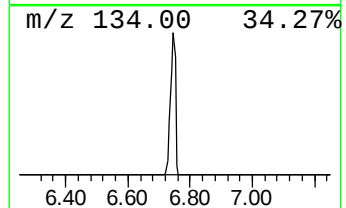
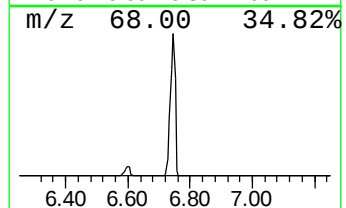
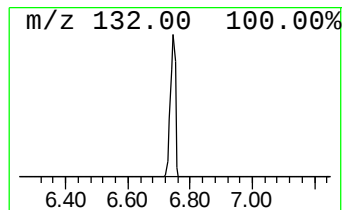
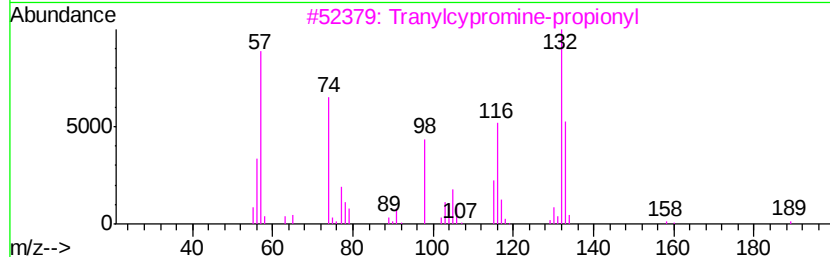
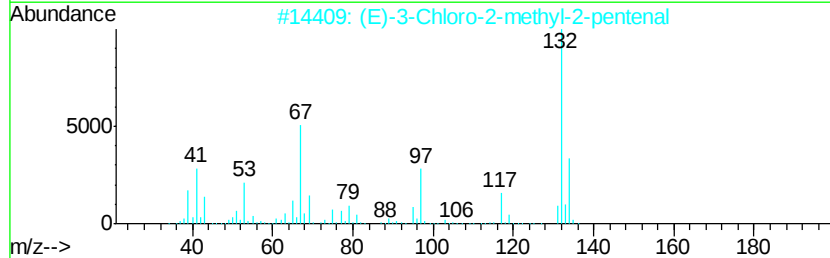
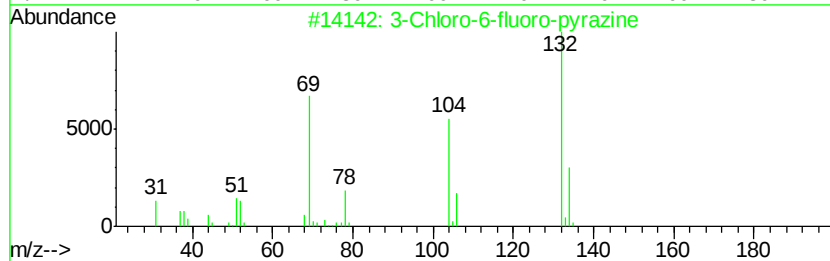
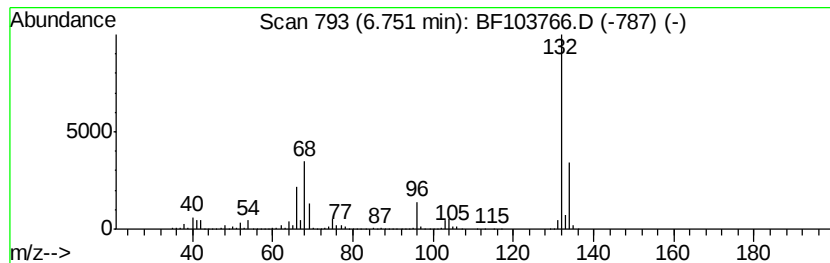
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	94.97 ng	4498300	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	16
3		Tranvlcyproline-propionyl	189	C12H15NO	1000123-86-3	10
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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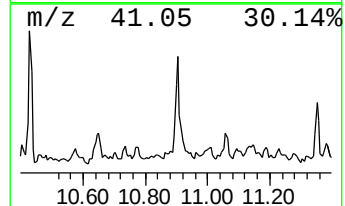
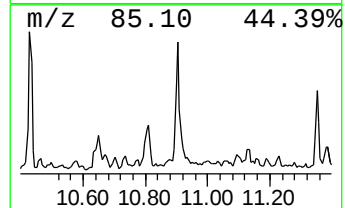
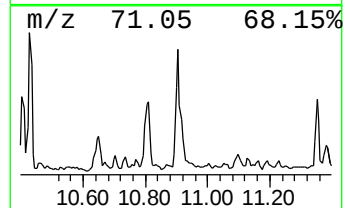
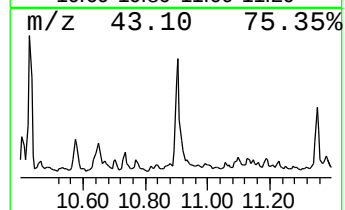
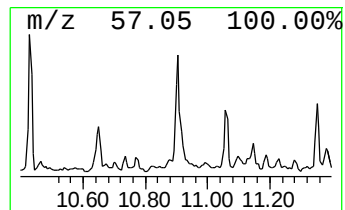
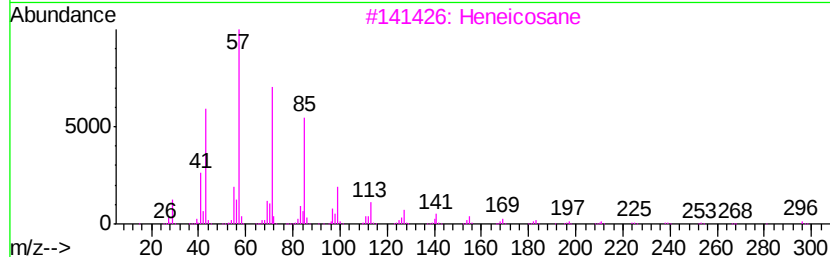
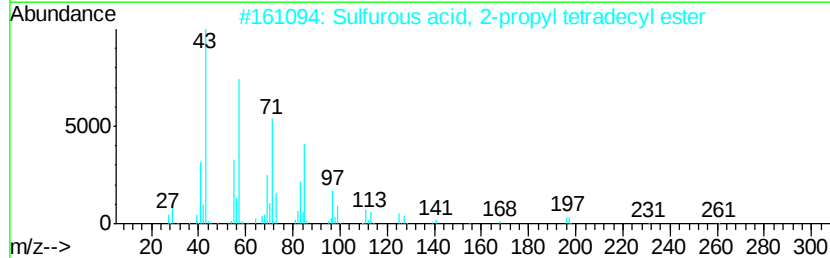
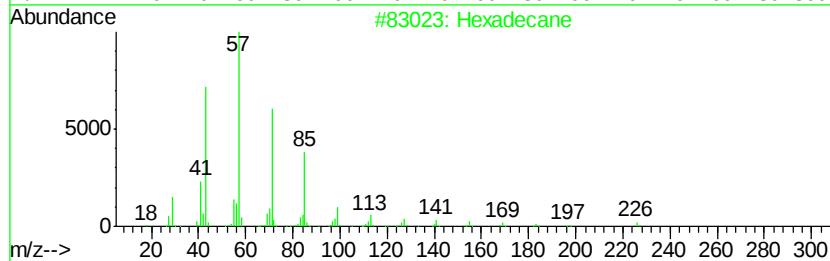
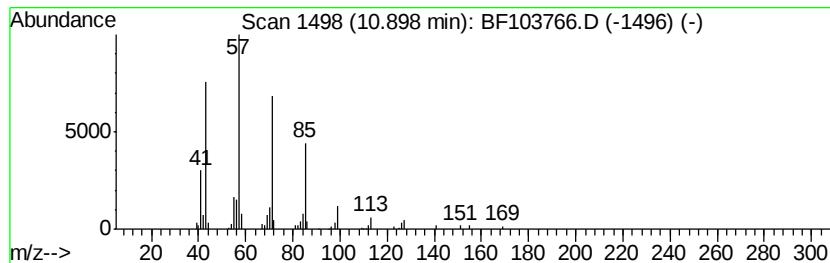
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Peak Number 5 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.56 ng	163765	Phenanthrene-d10	11.50

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Sulfurous acid, 2-propyl tetradec...		320	C17H36O3S	1000309-12-5	90
3	Heneicosane		296	C21H44	000629-94-7	90
4	Tetradecane		198	C14H30	000629-59-4	90
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	86



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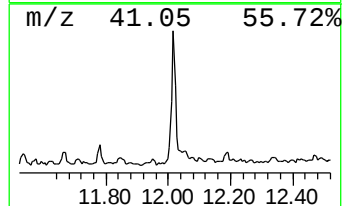
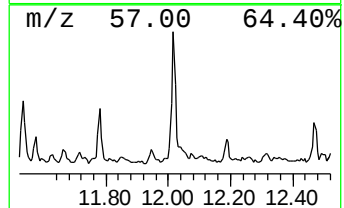
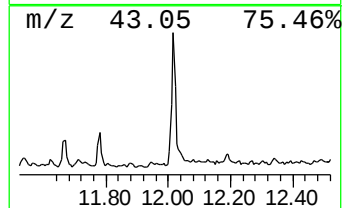
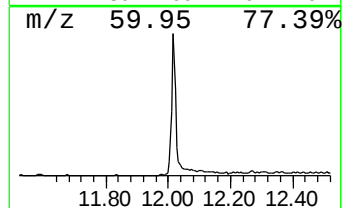
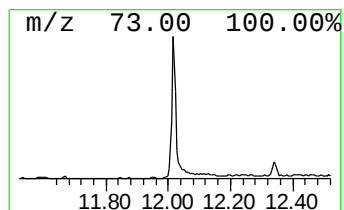
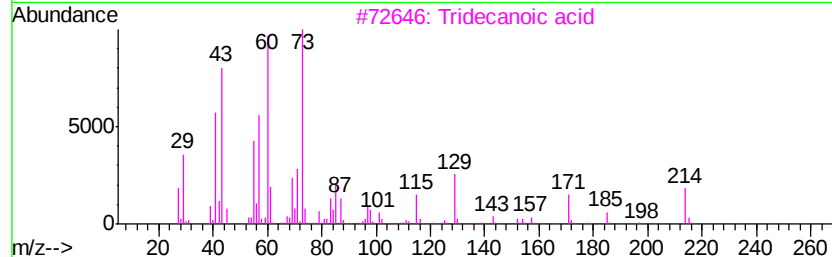
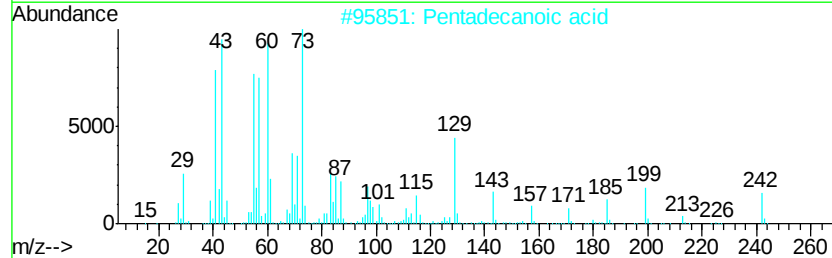
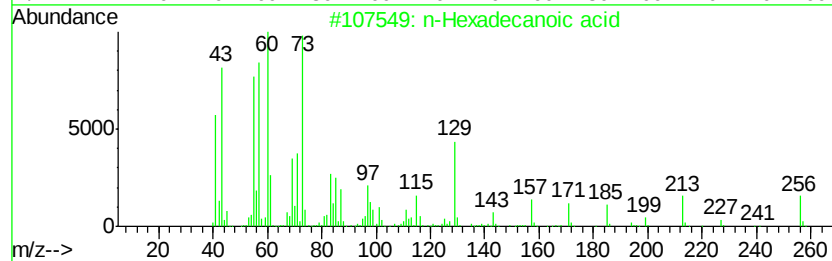
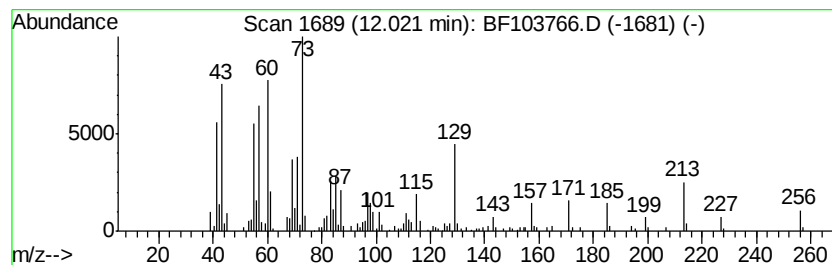
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	6.15 ng	393402	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
Data File : BF103766.D
Acq On : 19 Mar 2018 20:03
Operator : JU/SJ
Sample : J1971-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

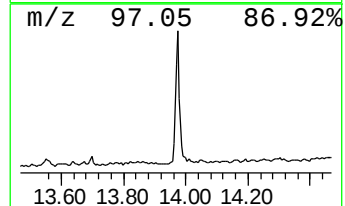
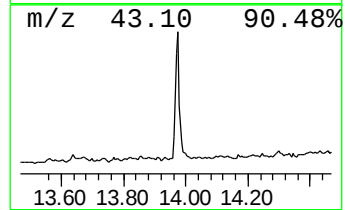
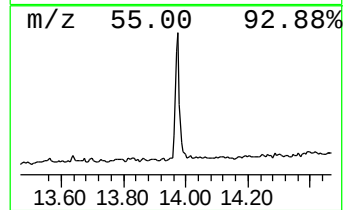
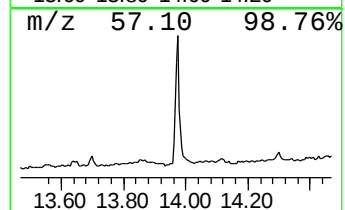
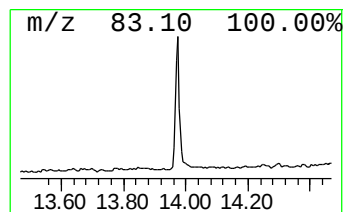
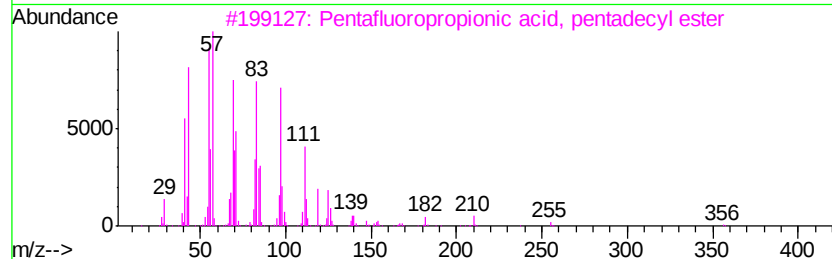
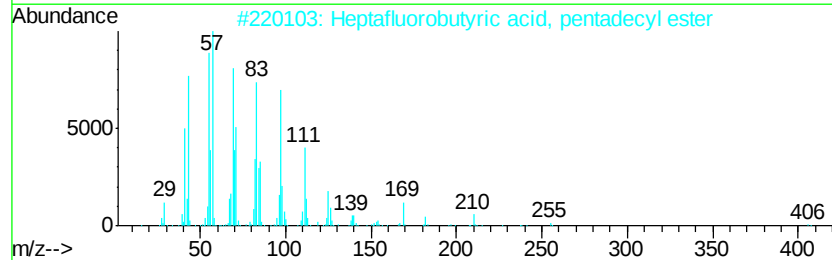
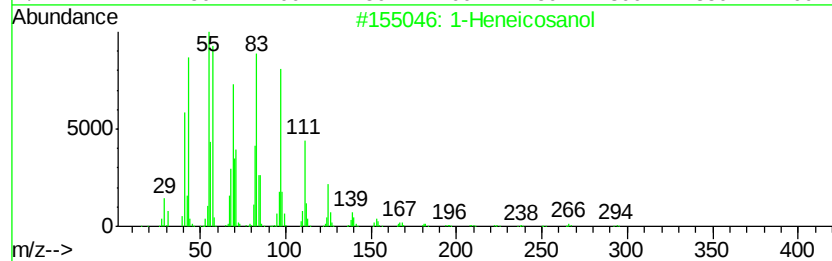
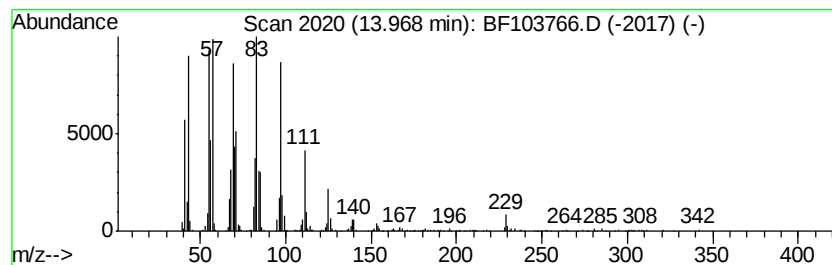
Instrument :
BNA_F
ClientSampleId :
ES-6-SA-2-EW@3

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 7 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.97	11.20 ng	593604	Chrysene-d12	14.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94



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Acq On : 19 Mar 2018 20:03
Operator : JU/SJ
Sample : J1971-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ES-6-SA-2-EW@3

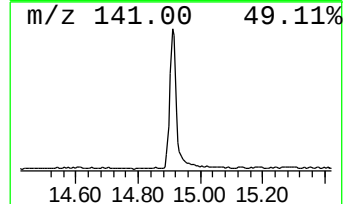
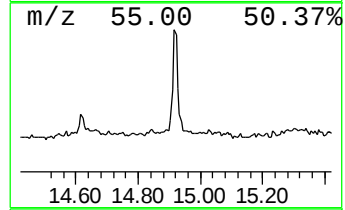
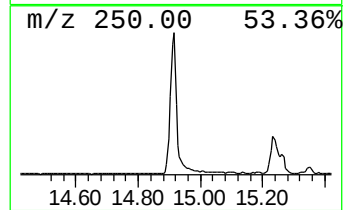
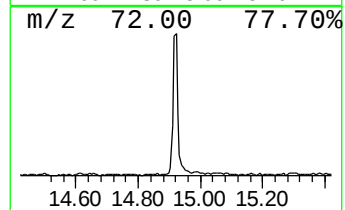
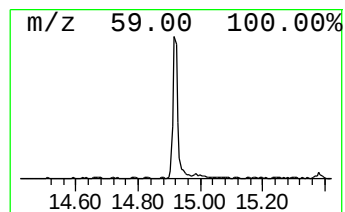
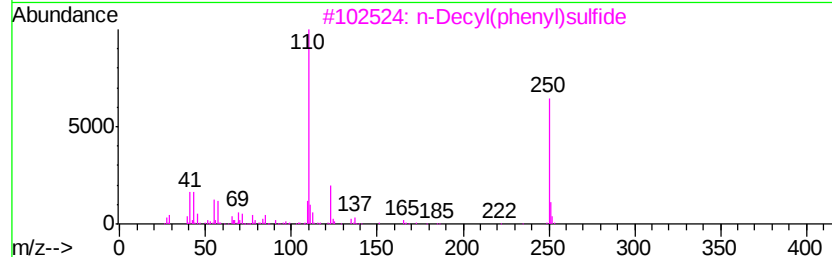
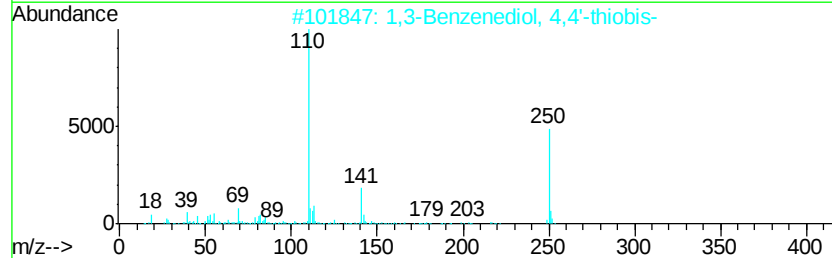
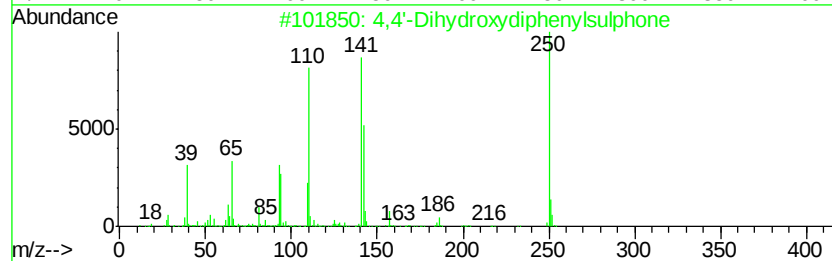
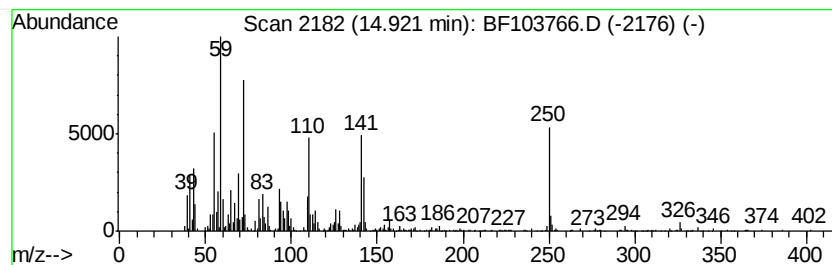
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.92	17.48 ng	926664	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	99
2		1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	41
3		n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	25
4		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	15
5		1,3-Benzenediol, o-(2,6-difluoro...	250	C13H8F2O3	1000330-83-2	10



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Sample : J1971-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ES-6-SA-2-EW@3

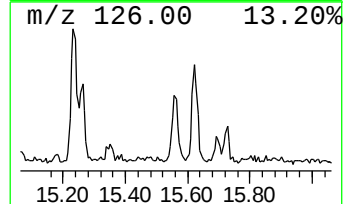
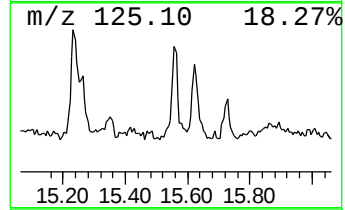
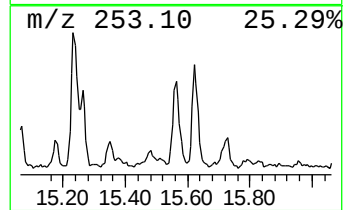
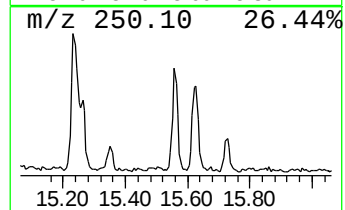
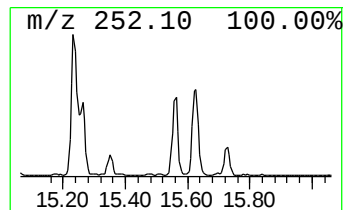
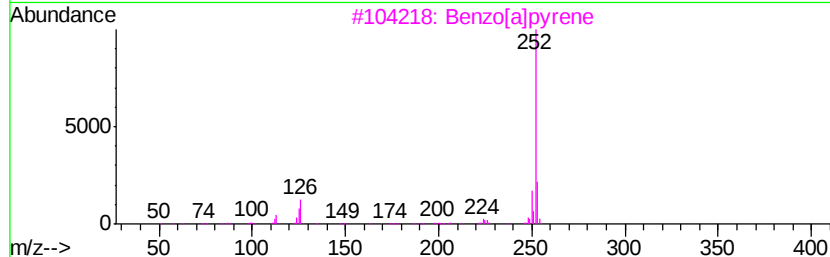
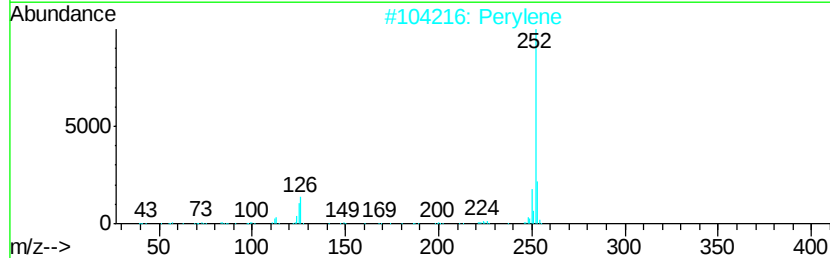
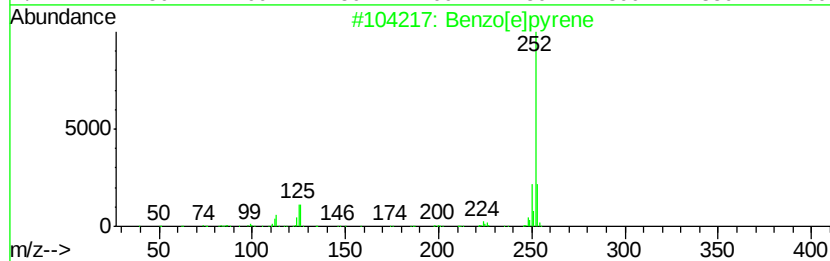
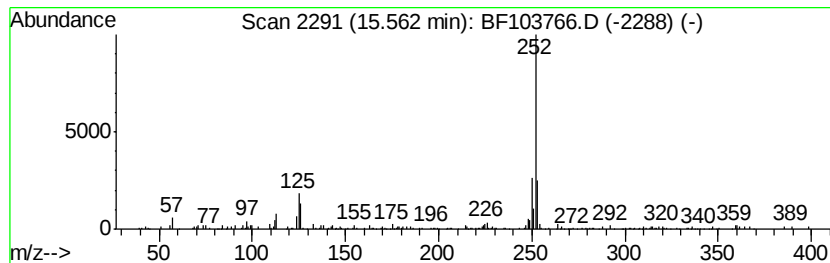
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.56	3.04 ng	120826	Perylene-d12	15.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2		Perylene	252	C20H12	000198-55-0	93
3		Benzo[a]pyrene	252	C20H12	000050-32-8	93
4		Benzo[e]acephenanthrylene	252	C20H12	000205-99-2	89
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	89



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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ES-6-SA-2-EW@3

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...	2.33	5.1 ng		241410	1	6.97	947288	20.0
2-Pentanone, 4-hy...	5.23	5.8 ng		274213	1	6.97	947288	20.0
unknown6.75	6.75	95.0 ng		4498300	1	6.97	947288	20.0
Hexadecane	10.90	2.6 ng		163765	4	11.50	1278490	20.0
n-Hexadecanoic acid	12.02	6.2 ng		393402	4	11.50	1278490	20.0
1-Heneicosanol	13.97	11.2 ng		593604	5	14.16	1059980	20.0
4,4'-Dihydroxydip...	14.92	17.5 ng		926664	5	14.16	1059980	20.0
Benzo[e]pyrene	15.56	3.0 ng		120826	6	15.70	794355	20.0