

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
 Data File : BF104899.D
 Acq On : 27 Apr 2018 23:19
 Operator : JU/SJ
 Sample : J2549-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

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-BF040618.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

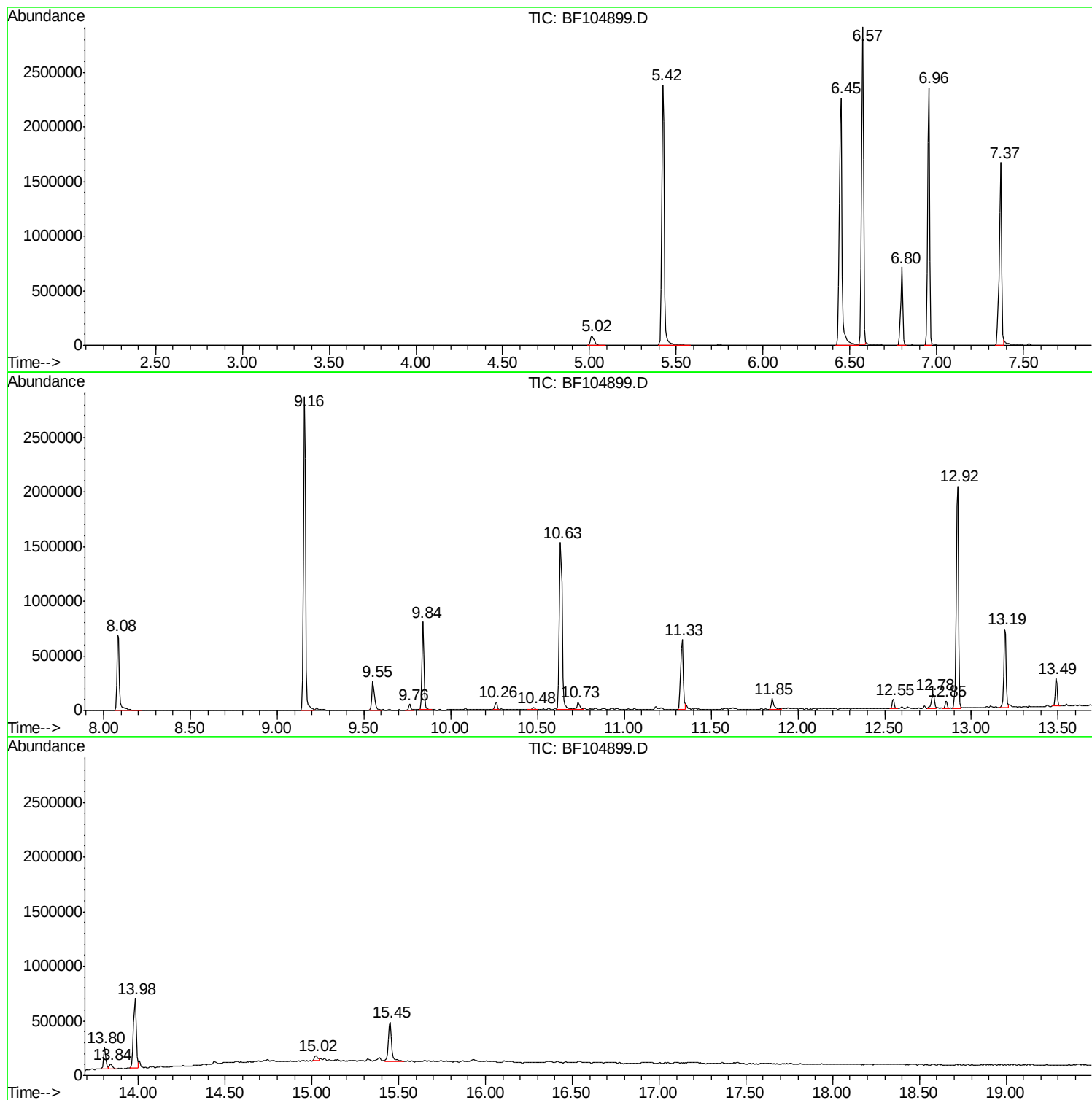
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	493	498	510	rVB	85964	121538	4.59%	0.515%
2	5.422	563	567	594	rBV	2388292	2609994	98.58%	11.058%
3	6.451	736	742	759	rBV	2269003	2647568	100.00%	11.217%
4	6.575	759	763	766	rBV	2907690	2632310	99.42%	11.153%
5	6.798	797	801	805	rBV	714351	564918	21.34%	2.394%
6	6.957	823	828	831	rBV	2359850	2050806	77.46%	8.689%
7	7.369	893	898	901	rBV	1674467	1570354	59.31%	6.653%
8	8.081	1016	1019	1042	rVB	689209	726996	27.46%	3.080%
9	9.157	1198	1202	1212	rBV	2872405	2634935	99.52%	11.164%
10	9.551	1266	1269	1277	rVB	263756	248314	9.38%	1.052%
11	9.763	1301	1305	1309	rBV	53885	46217	1.75%	0.196%
12	9.839	1314	1318	1326	rVV2	804983	723912	27.34%	3.067%
13	10.263	1387	1390	1392	rVB	72453	57583	2.17%	0.244%
14	10.480	1421	1427	1430	rBV2	22872	28432	1.07%	0.120%
15	10.633	1449	1453	1467	rBV	1528071	1514965	57.22%	6.419%
16	10.733	1467	1470	1475	rBV	65701	68591	2.59%	0.291%
17	11.333	1568	1572	1575	rBV	636289	615312	23.24%	2.607%
18	11.851	1657	1660	1669	rBV2	96188	105824	4.00%	0.448%
19	12.551	1775	1779	1783	rBV	84683	83281	3.15%	0.353%
20	12.780	1812	1818	1821	rBV	127072	133336	5.04%	0.565%
21	12.851	1827	1830	1834	rVB	67236	57722	2.18%	0.245%
22	12.921	1837	1842	1845	rBV	2032353	1977315	74.68%	8.378%
23	13.192	1882	1888	1892	rBV	717800	714194	26.98%	3.026%
24	13.486	1935	1938	1942	rVB	257365	218103	8.24%	0.924%
25	13.804	1989	1992	1996	rBV	195380	192399	7.27%	0.815%
26	13.839	1996	1998	2003	rVB	48903	54350	2.05%	0.230%
27	13.980	2017	2022	2025	rBV	634987	622520	23.51%	2.638%
28	15.021	2196	2199	2203	rBV	45643	67793	2.56%	0.287%
29	15.451	2267	2272	2285	rVB	359082	512560	19.36%	2.172%

Sum of corrected areas: 23602142

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.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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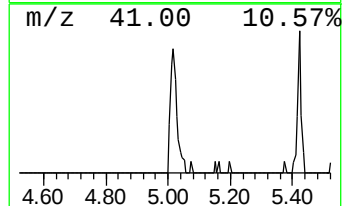
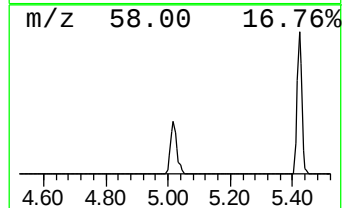
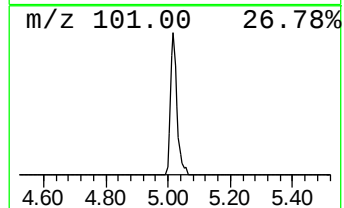
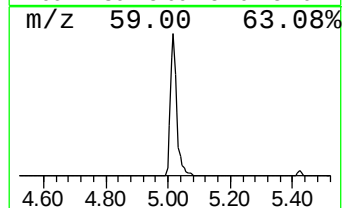
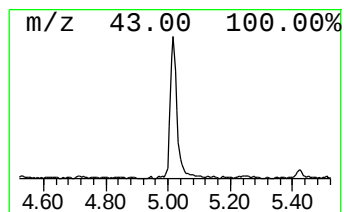
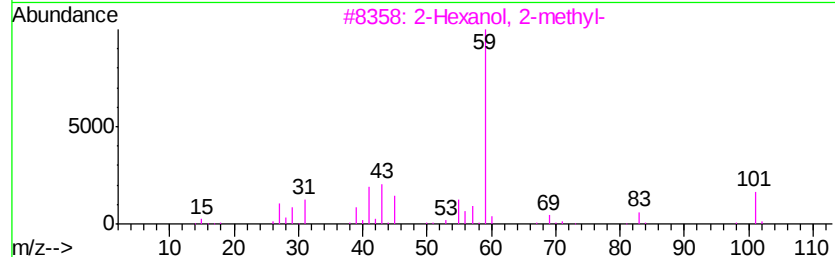
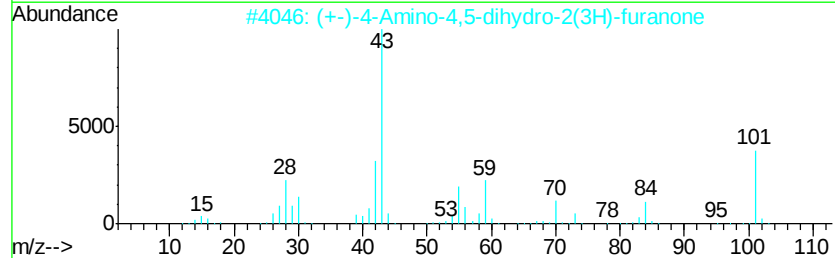
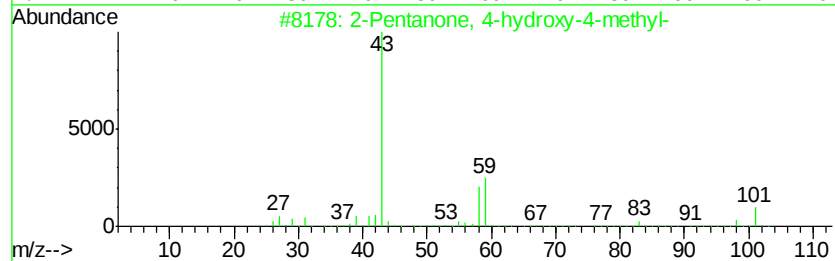
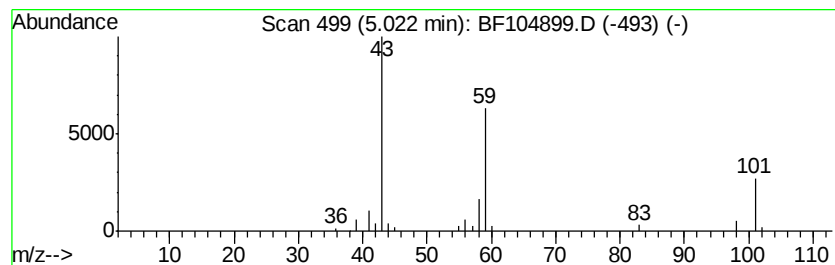
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.30 ng	121538	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	38
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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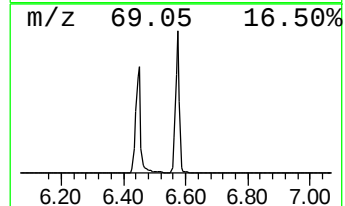
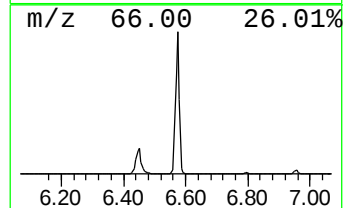
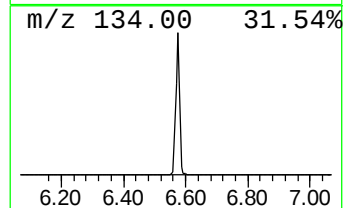
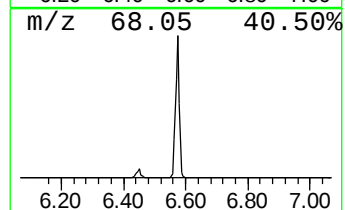
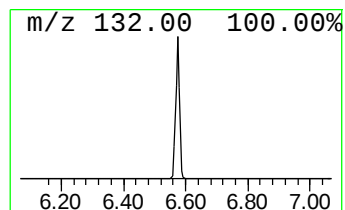
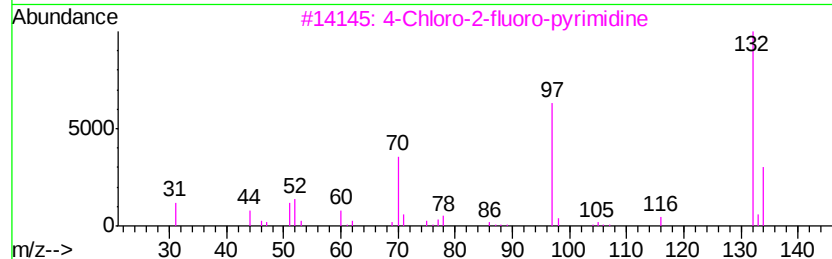
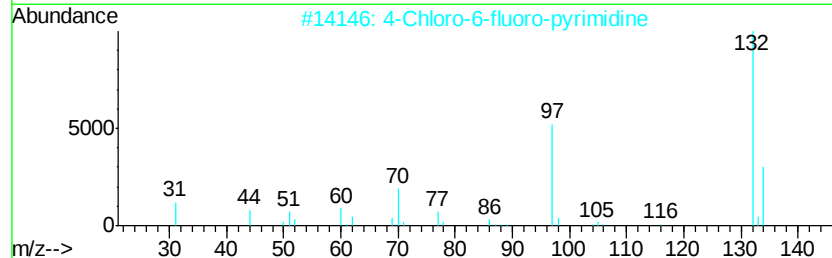
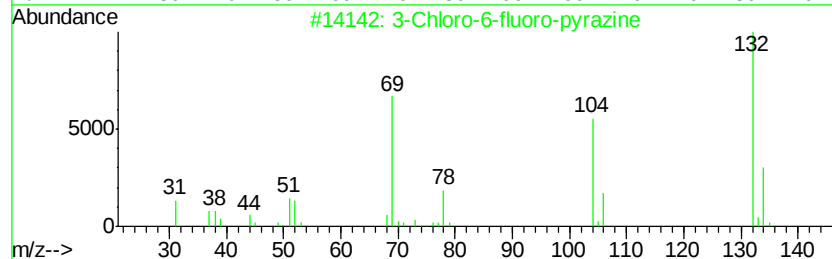
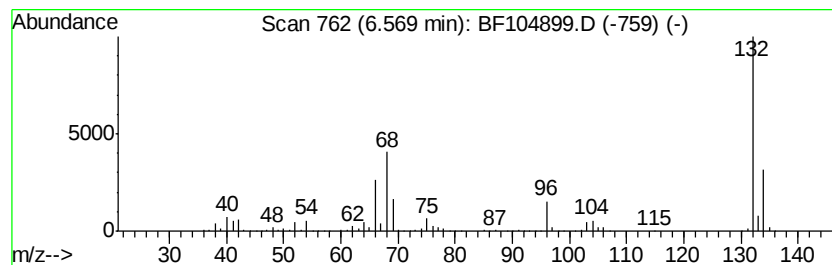
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	93.19 ng	2632310	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
3	4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5		5-Aminoindole	132	C8H8N2	005192-03-0	9
5	1		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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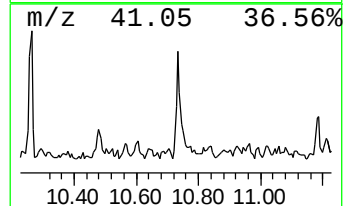
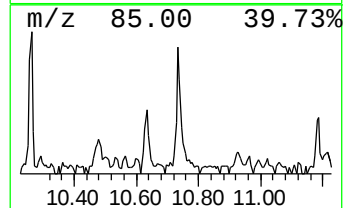
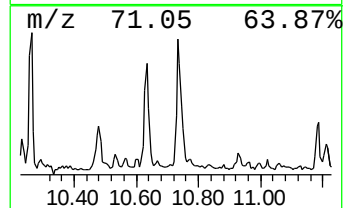
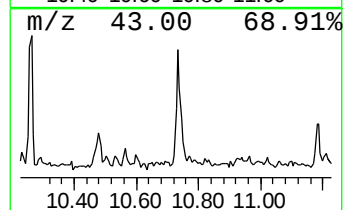
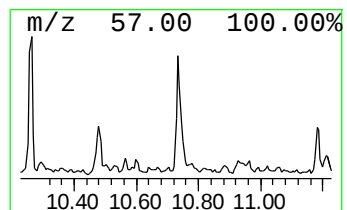
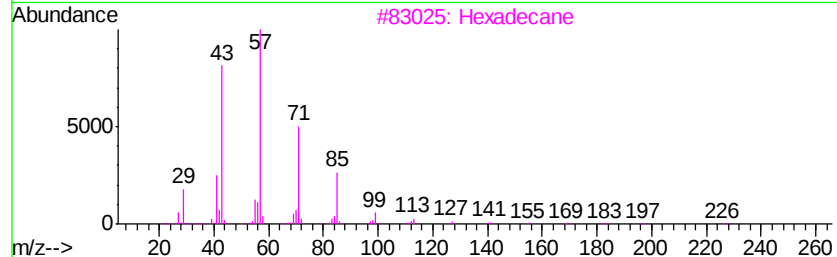
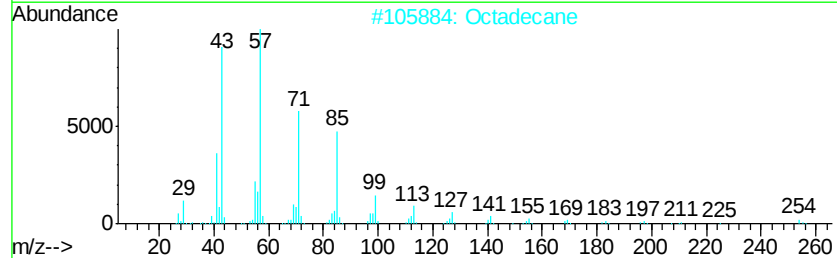
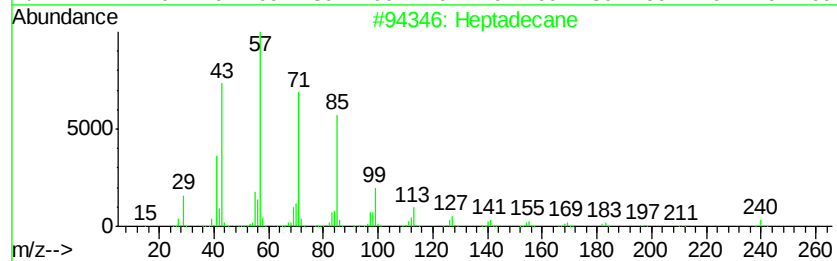
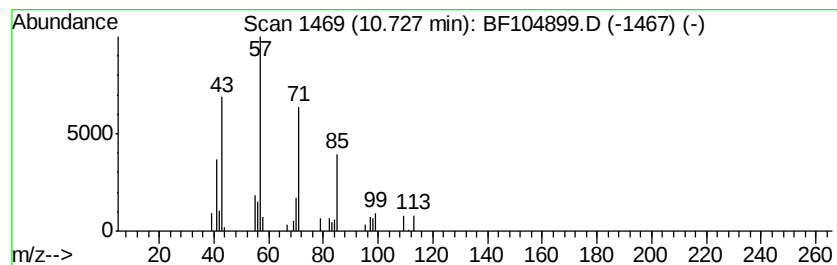
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.23 ng	68591	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Octadecane		254	C18H38	000593-45-3	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tetracosane		338	C24H50	000646-31-1	87
5	Sulfurous acid, 2-propyl tetrade...		320	C17H36O3S	1000309-12-5	86



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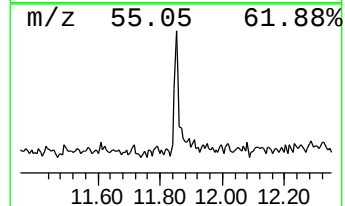
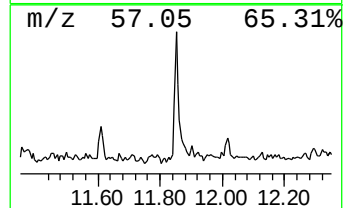
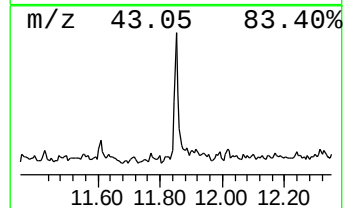
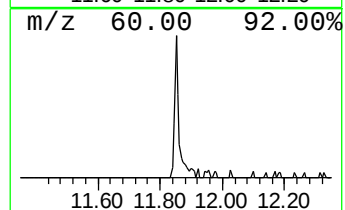
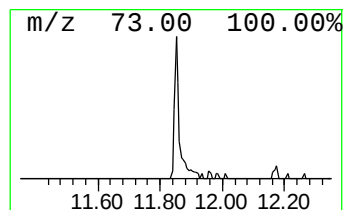
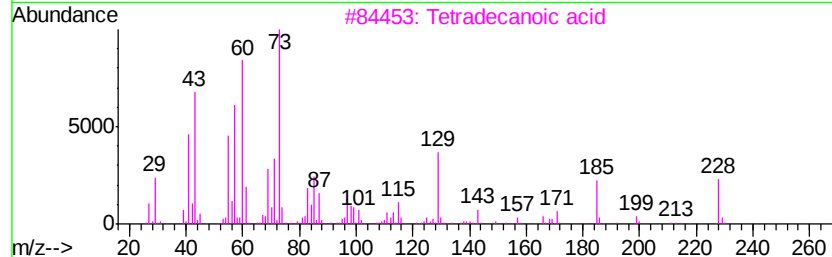
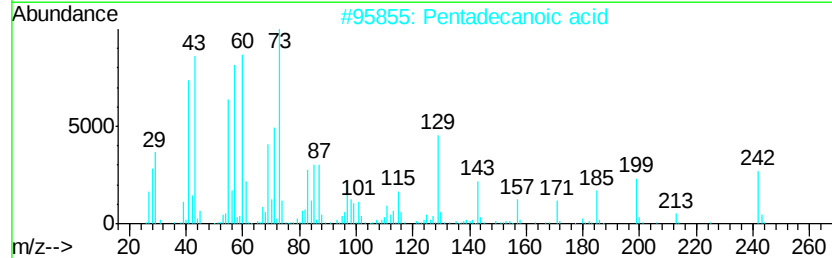
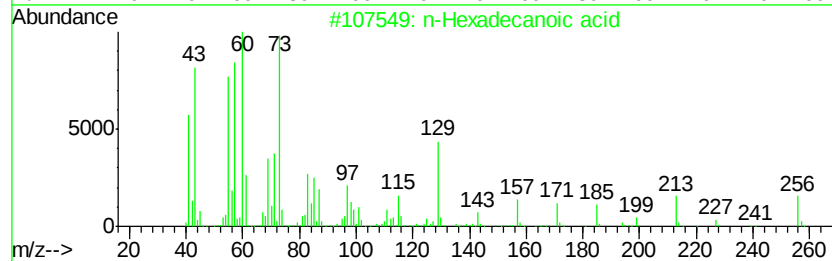
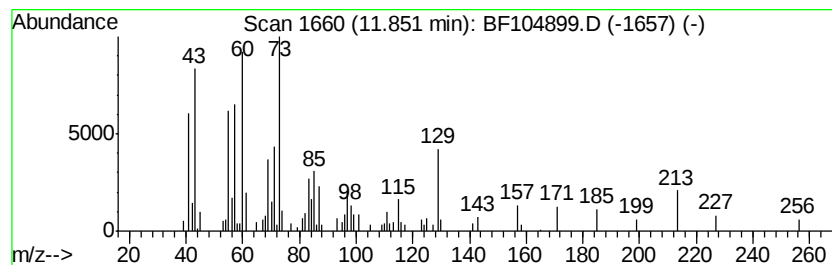
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	3.44 ng	105824	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



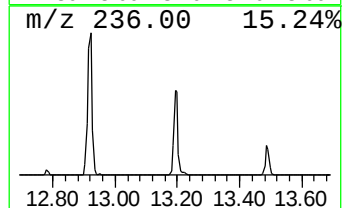
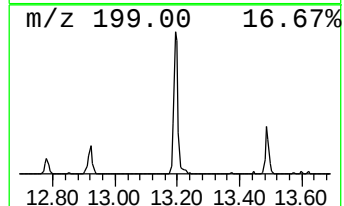
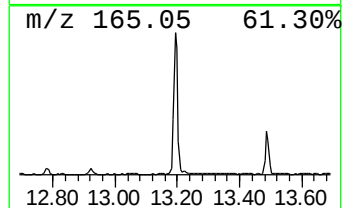
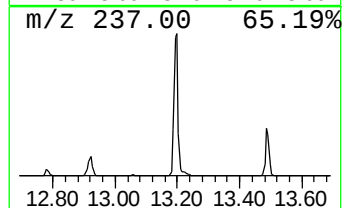
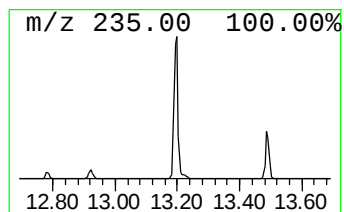
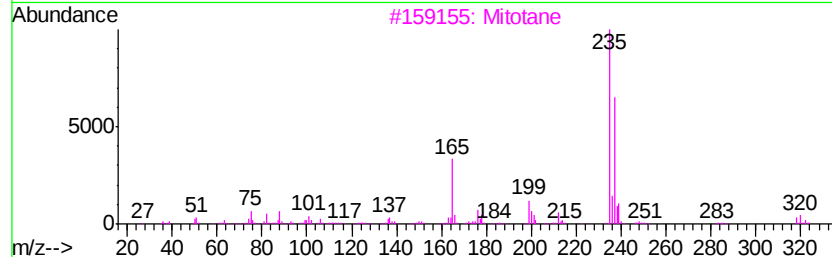
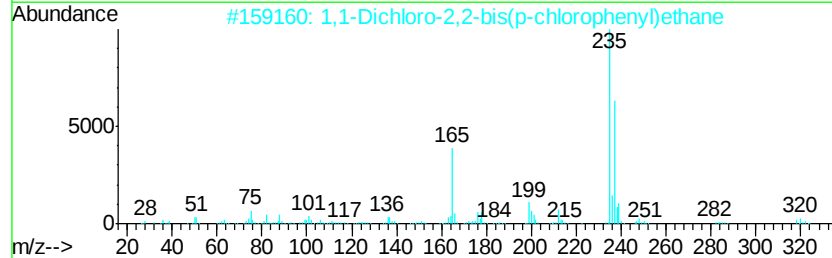
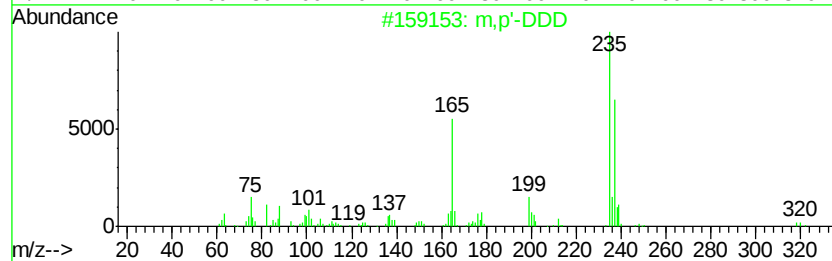
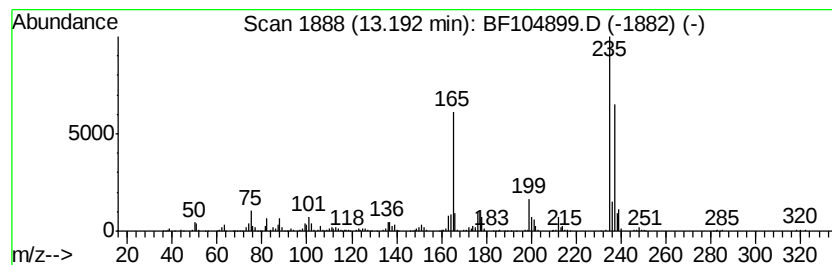
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Peak Number 6 m,p'-DDD Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	22.95 ng	714194	Chrysene-d12	13.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	m,p'-DDD		318 C14H10Cl4	004329-12-8 99
2	1,1-Dichloro-2,2-bis(p-chlorophe...		318 C14H10Cl4	000072-54-8 99
3	Mitotane		318 C14H10Cl4	000053-19-0 98
4	2,2-Bis(p-chlorophenyl)ethanol		266 C14H12Cl2O	002642-82-2 87
5	3-Butanone, 1,1-bis(4-chlorophen...		320 C18H18Cl2O	1000158-20-4 80



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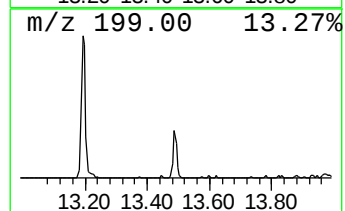
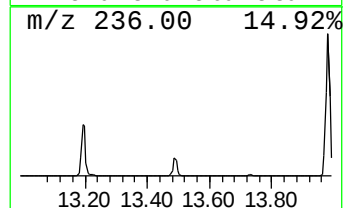
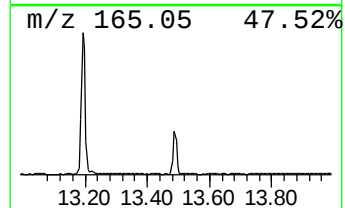
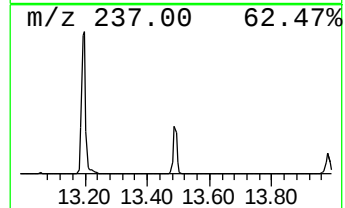
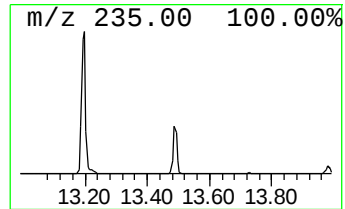
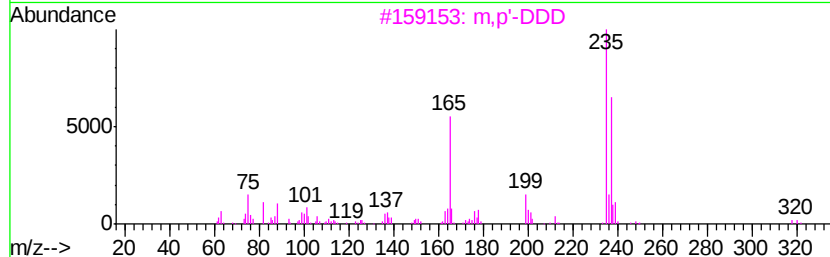
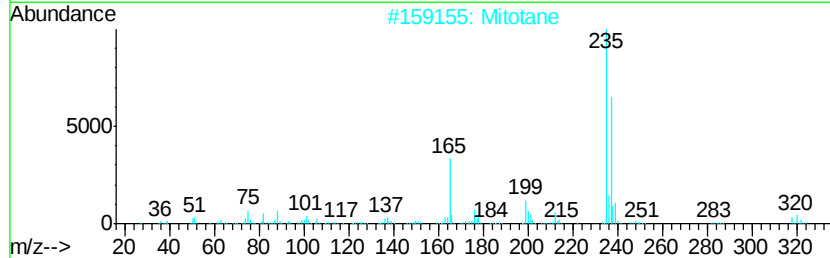
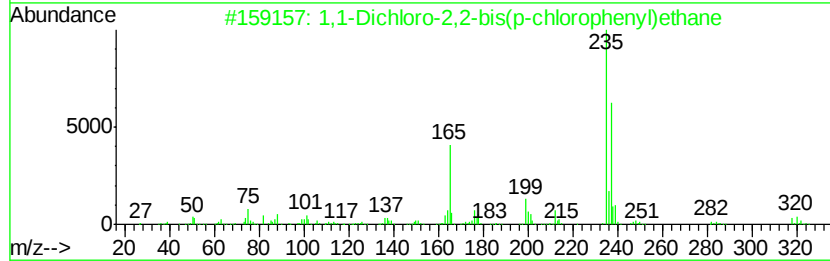
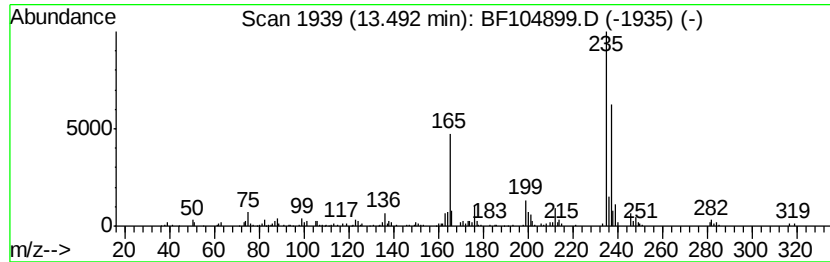
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,1-Dichloro-2,2-bis(p-chlo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	7.01 ng	218103	Chrysene-d12	13.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	91
2			Mitotane	318	C14H10Cl4	000053-19-0	91
3			m,p'-DDD	318	C14H10Cl4	004329-12-8	90
4			p,p'-DDT	352	C14H9Cl5	000050-29-3	90
5			2,2-Bis(p-chlorophenyl)ethanol	266	C14H12Cl2O	002642-82-2	83



Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
Data File : BF104899.D
Acq On : 27 Apr 2018 23:19
Operator : JU/SJ
Sample : J2549-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

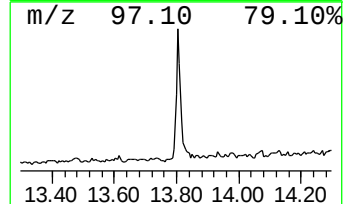
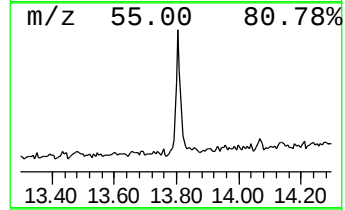
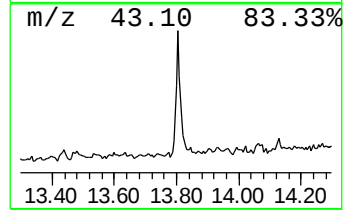
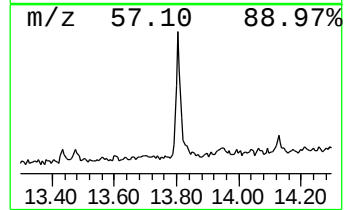
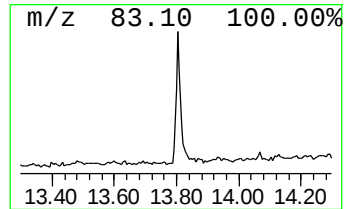
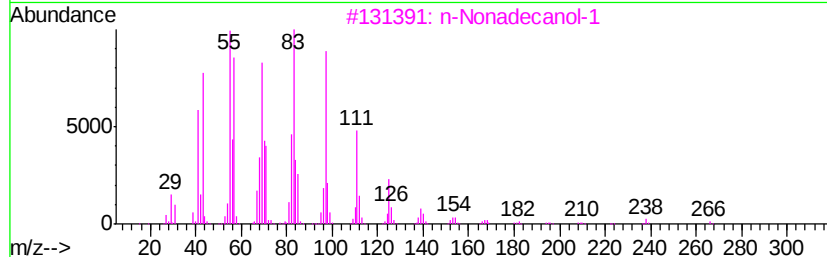
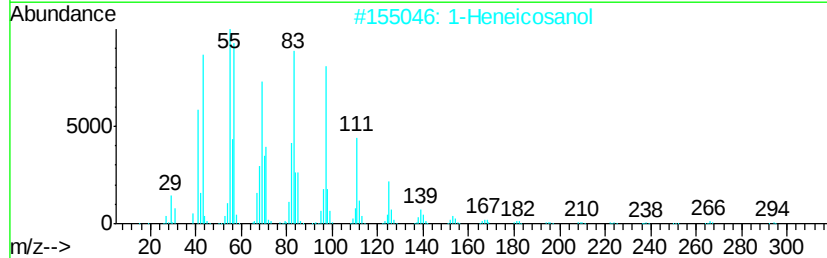
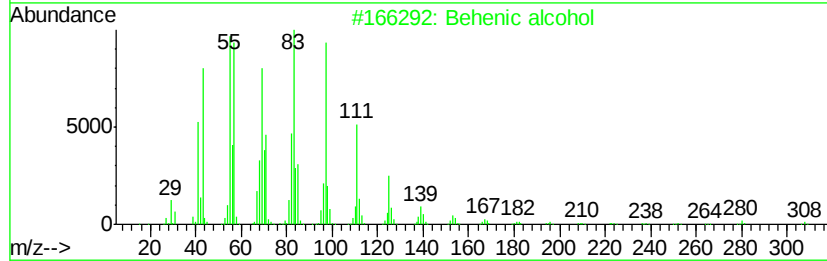
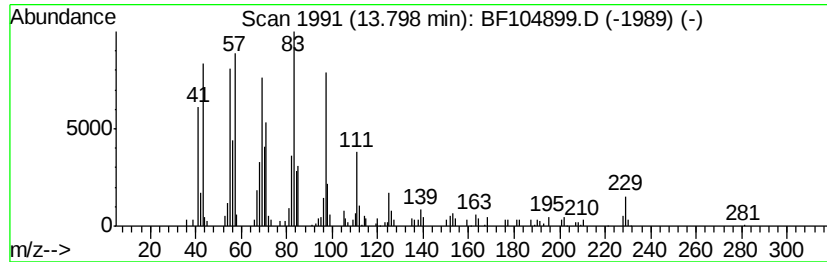
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	6.18 ng	192399	Chrysene-d12	13.98

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104899.D
Acq On : 27 Apr 2018 23:19
Operator : JU/SJ
Sample : J2549-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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
2-Pentanone, 4-hy...	5.02	4.3	ng	121538	1	6.80	564918	20.0
unknown6.57	6.57	93.2	ng	2632310	1	6.80	564918	20.0
Heptadecane	10.73	2.2	ng	68591	4	11.33	615312	20.0
n-Hexadecanoic acid	11.85	3.4	ng	105824	4	11.33	615312	20.0
m,p'-DDD	13.19	22.9	ng	714194	5	13.98	622520	20.0
1,1-Dichloro-2,2-...	13.49	7.0	ng	218103	5	13.98	622520	20.0
Behenic alcohol	13.80	6.2	ng	192399	5	13.98	622520	20.0