

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
 Data File : BF104902.D
 Acq On : 28 Apr 2018 00:39
 Operator : JU/SJ
 Sample : J2590-02
 Misc :
 ALS Vial : 24 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

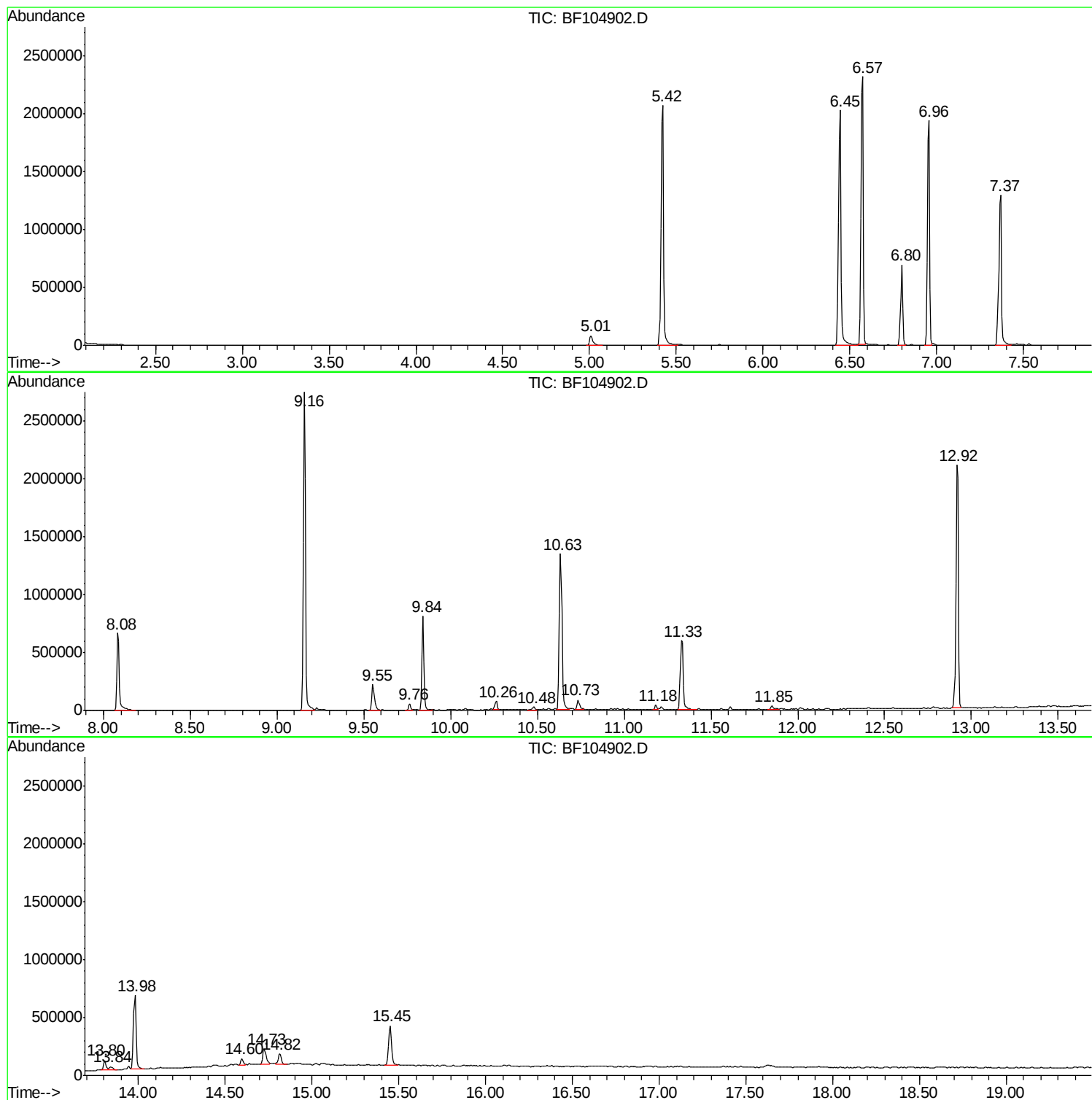
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	492	497	508	rBV	84308	115105	4.61%	0.565%
2	5.422	562	567	582	rBV	2068315	2175031	87.10%	10.681%
3	6.445	736	741	758	rBV	2030513	2201576	88.16%	10.812%
4	6.575	758	763	766	rBV	2315269	2245325	89.92%	11.026%
5	6.798	797	801	805	rBV	694549	541996	21.70%	2.662%
6	6.957	823	828	831	rBV	1940812	1796086	71.93%	8.820%
7	7.369	893	898	908	rBV	1295505	1354172	54.23%	6.650%
8	8.081	1016	1019	1036	rBV	667605	688449	27.57%	3.381%
9	9.157	1198	1202	1212	rBV	2748478	2497139	100.00%	12.263%
10	9.551	1265	1269	1276	rBV	224866	218333	8.74%	1.072%
11	9.763	1301	1305	1308	rBV	56371	47276	1.89%	0.232%
12	9.839	1314	1318	1327	rBV	809633	690556	27.65%	3.391%
13	10.263	1387	1390	1392	rVB	71520	60416	2.42%	0.297%
14	10.480	1421	1427	1430	rBV	24642	33671	1.35%	0.165%
15	10.633	1449	1453	1462	rBV	1345316	1298152	51.99%	6.375%
16	10.733	1467	1470	1475	rBV	81442	82881	3.32%	0.407%
17	11.180	1543	1546	1549	rBV	37158	33463	1.34%	0.164%
18	11.327	1568	1571	1586	rBV	595269	632717	25.34%	3.107%
19	11.851	1656	1660	1667	rBV2	29977	34266	1.37%	0.168%
20	12.916	1837	1841	1845	rBV	2096396	2084650	83.48%	10.237%
21	13.804	1989	1992	1996	rBV	83293	93270	3.74%	0.458%
22	13.839	1996	1998	2004	rVB	29808	35553	1.42%	0.175%
23	13.980	2018	2022	2031	rBV	638187	608538	24.37%	2.988%
24	14.598	2124	2127	2130	rBV	58289	56626	2.27%	0.278%
25	14.727	2145	2149	2154	rBV	128578	158276	6.34%	0.777%
26	14.815	2160	2164	2171	rVB2	93652	125160	5.01%	0.615%
27	15.451	2267	2272	2279	rBV	341026	454407	18.20%	2.232%

Sum of corrected areas: 20363090

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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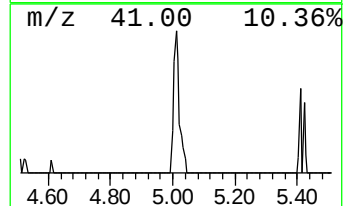
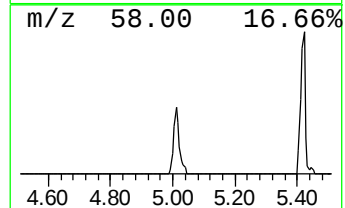
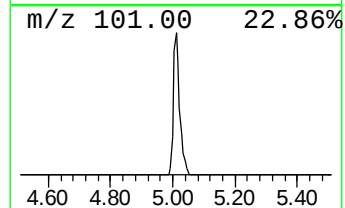
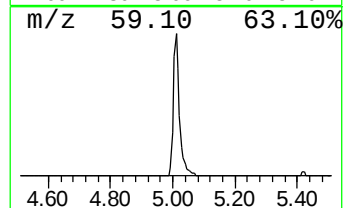
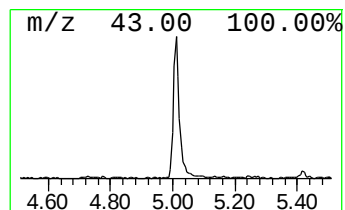
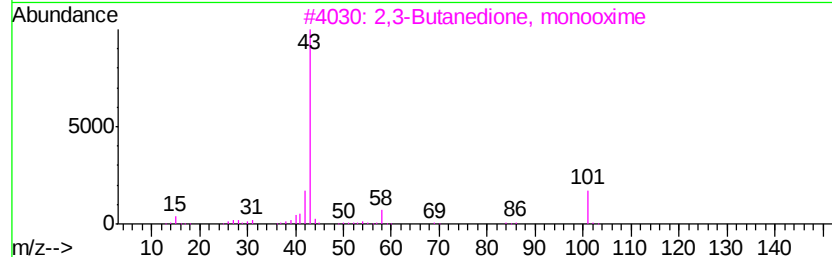
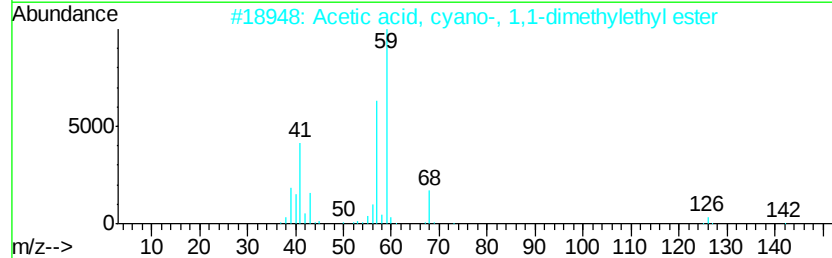
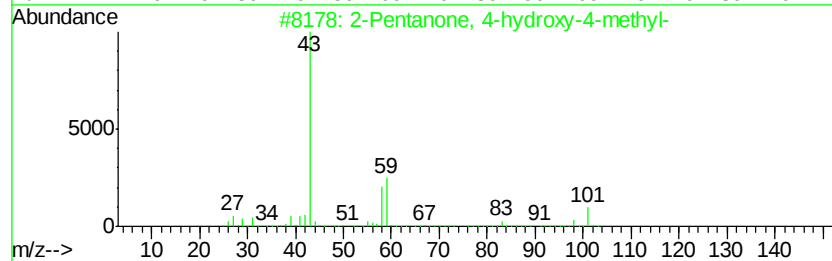
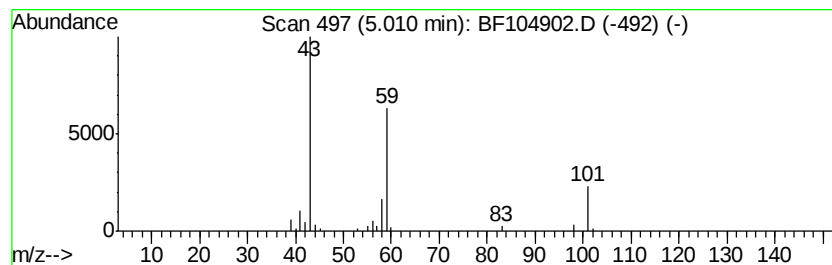
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	4.25 ng	115105	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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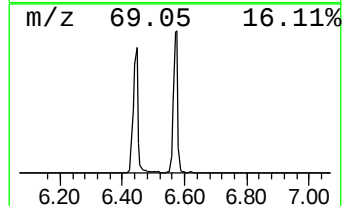
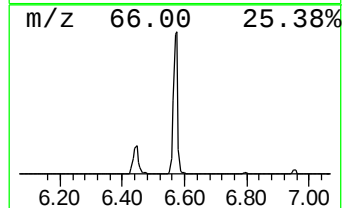
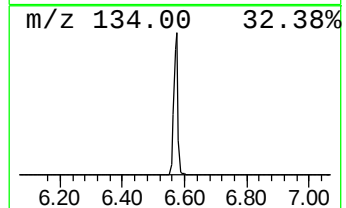
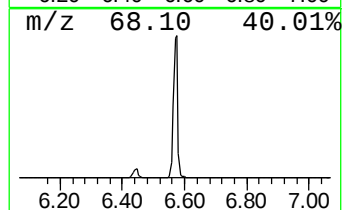
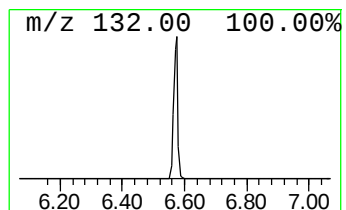
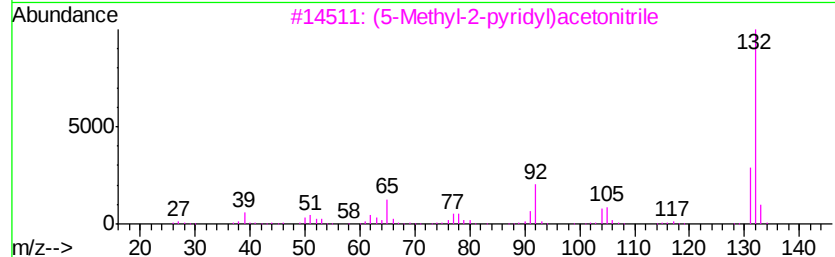
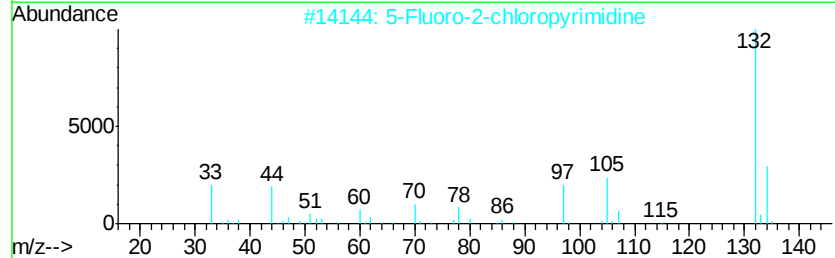
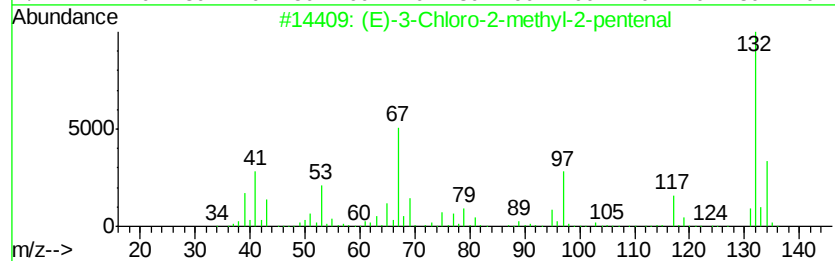
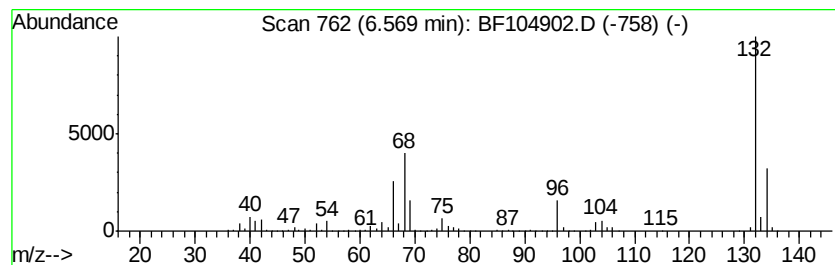
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	82.85 ng	2245330	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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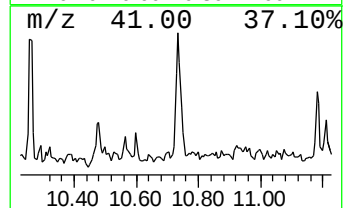
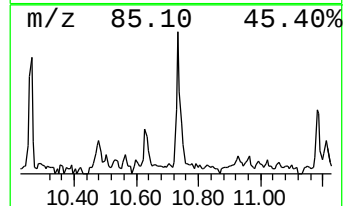
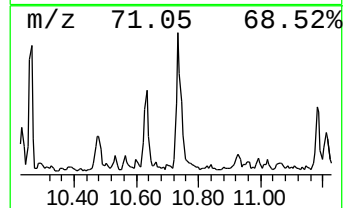
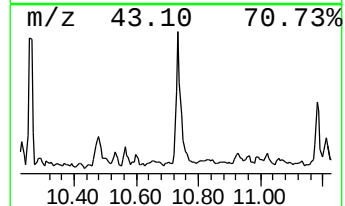
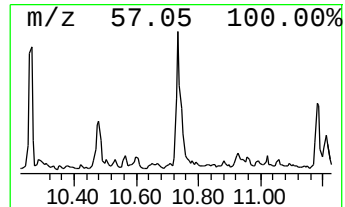
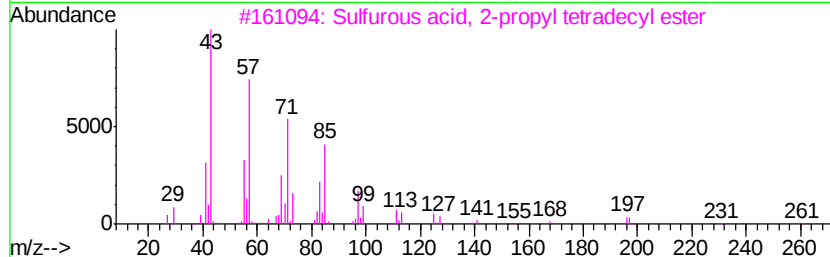
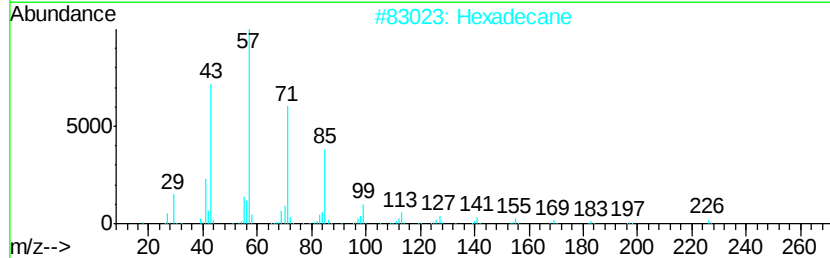
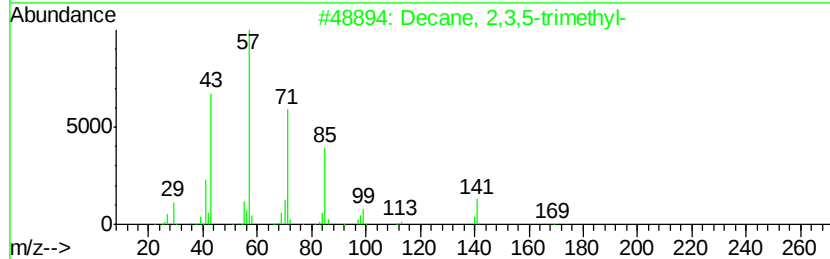
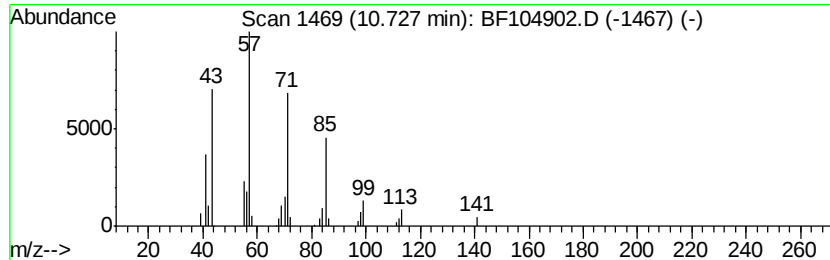
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Peak Number 4 Decane, 2,3,5-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	2.62 ng	82881	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
2		Hexadecane	226	C16H34	000544-76-3	86
3		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	78
4		Heneicosane	296	C21H44	000629-94-7	72
5		Octacosane	394	C28H58	000630-02-4	72



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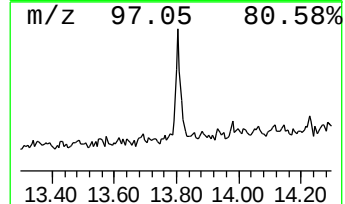
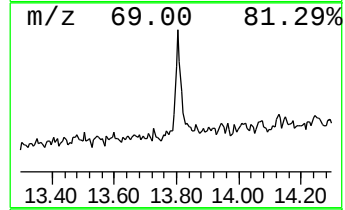
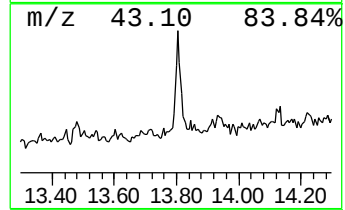
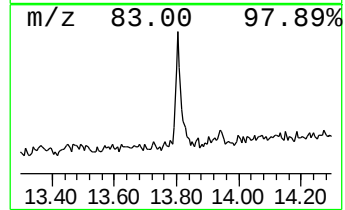
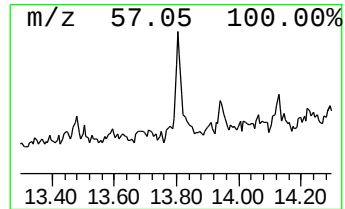
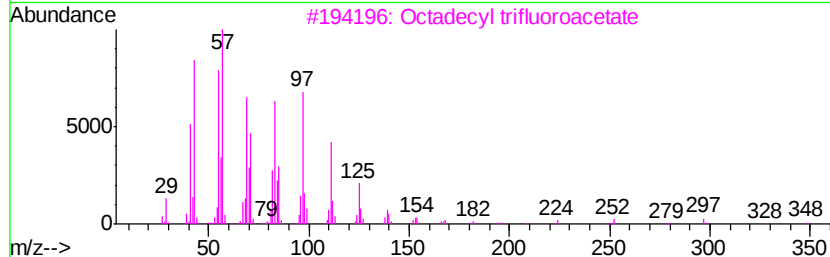
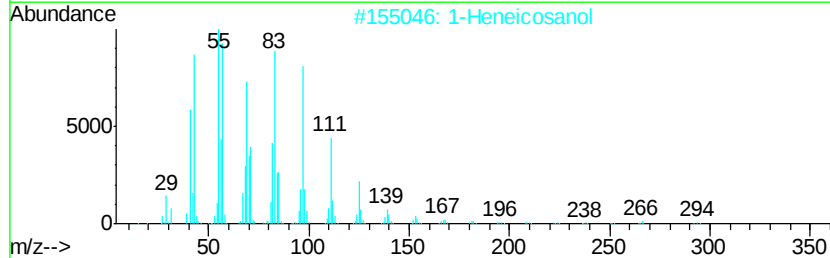
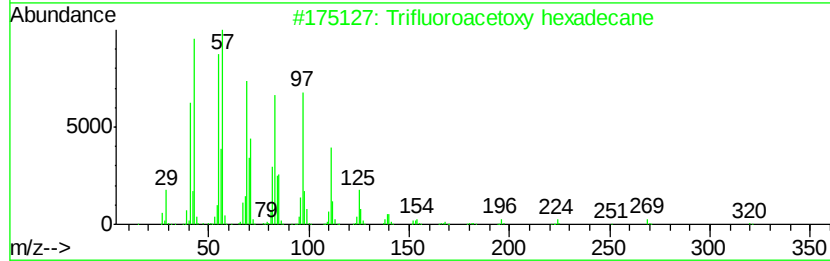
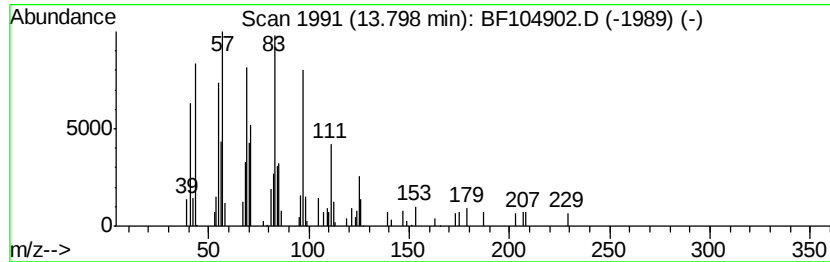
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	3.07 ng	93270	Chrysene-d12	13.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	76
2	1-Heneicosanol	312	C21H44O	015594-90-8	76
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	70
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	68



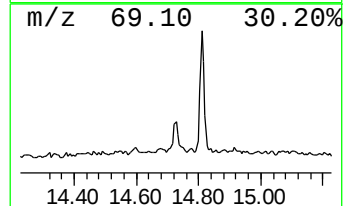
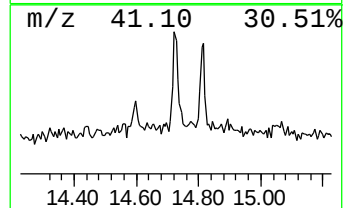
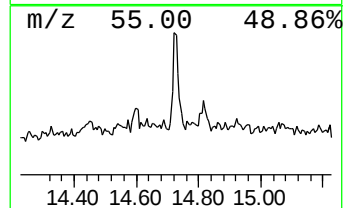
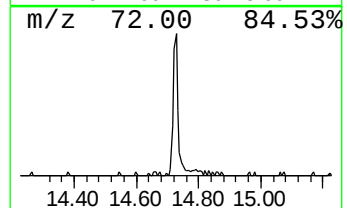
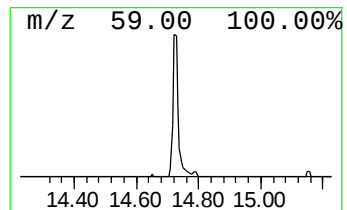
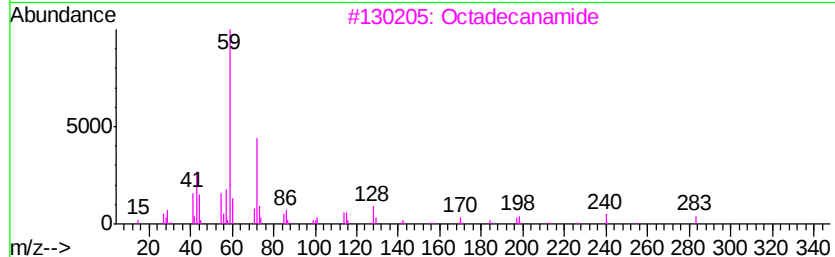
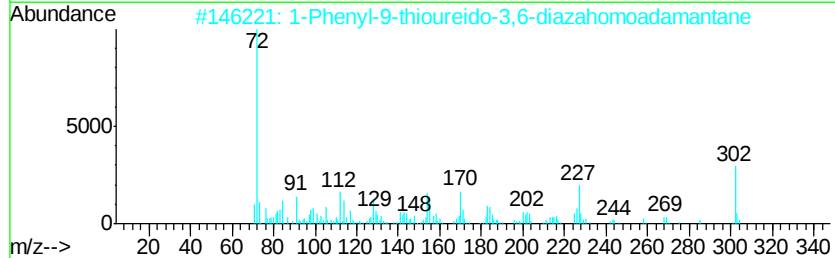
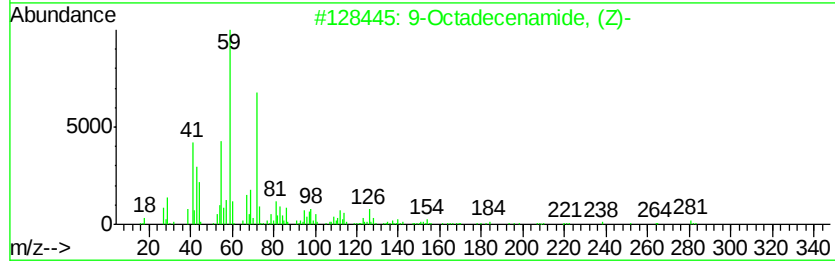
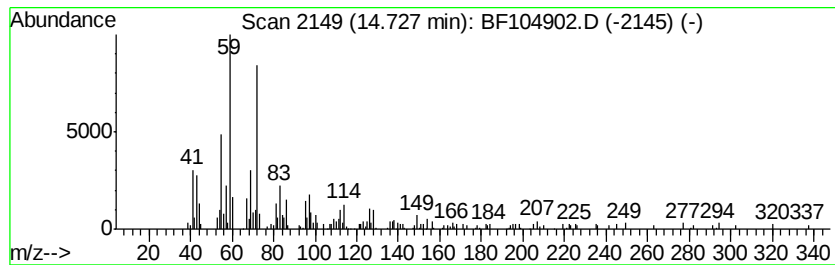
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.73	6.97 ng	158276	Perylene-d12	15.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	1-Phenyl-9-thioureido-3,6-diazah...	302	C16H22N4S	153464-71-2	50
3	Octadecanamide	283	C18H37NO	000124-26-5	47
4	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	35
5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	27



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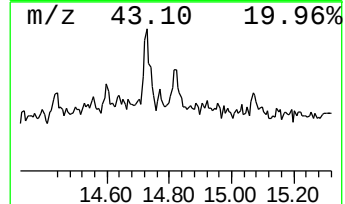
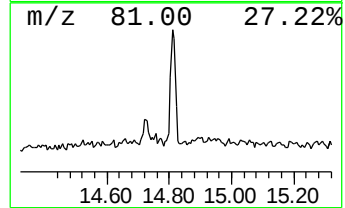
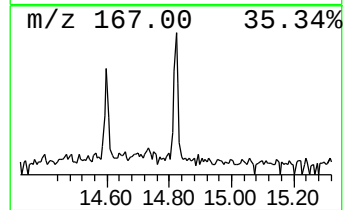
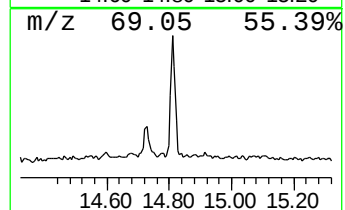
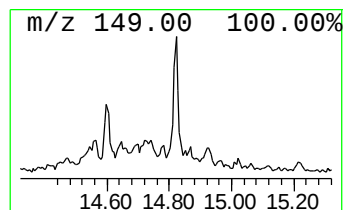
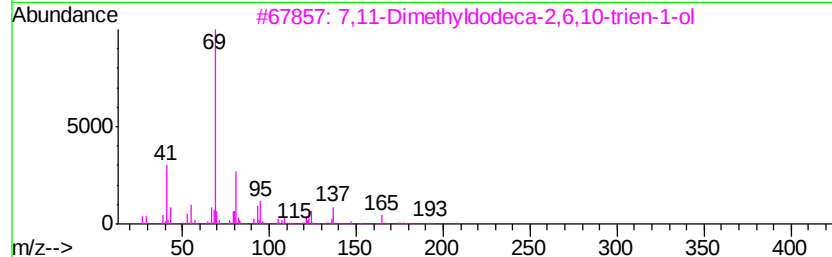
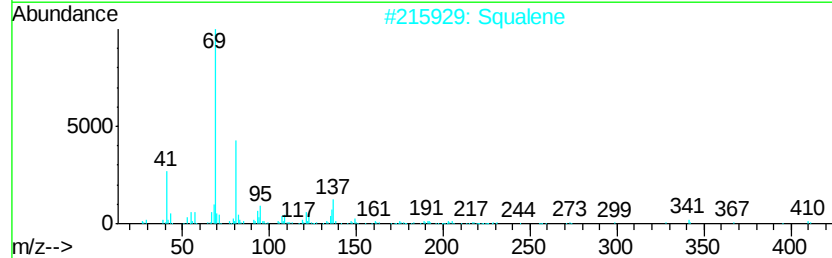
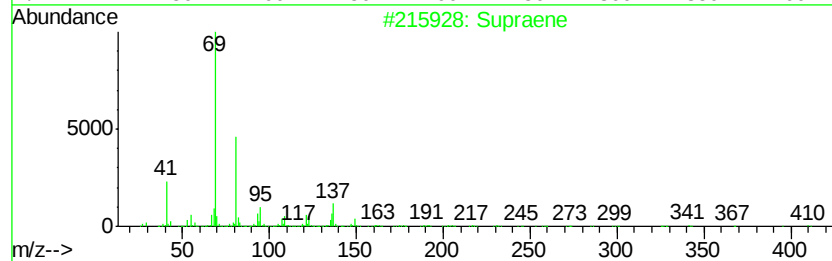
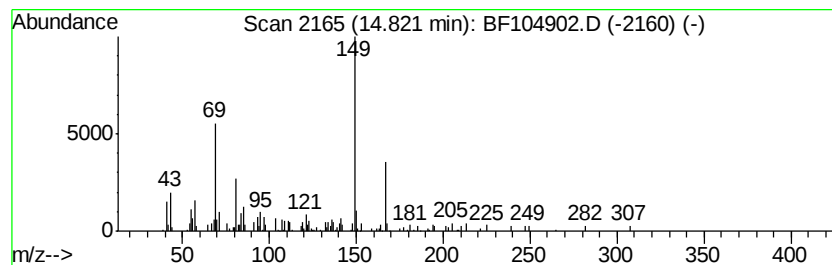
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	5.51 ng	125160	Perylene-d12	15.45

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	62
2	Squalene		410	C30H50	000111-02-4	58
3	7,11-Dimethyldodeca-2,6,10-trien...		208	C14H24O	125529-10-4	49
4	6,11-Dimethyl-2,6,10-dodecatrien...		208	C14H24O	1000196-53-3	49
5	trans-Farnesol		222	C15H26O	000106-28-5	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042718\
Data File : BF104902.D
Acq On : 28 Apr 2018 00:39
Operator : JU/SJ
Sample : J2590-02
Misc :
ALS Vial : 24 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...	5.01	4.3	ng	115105	1	6.80	541996	20.0
unknown6.57	6.57	82.8	ng	2245330	1	6.80	541996	20.0
Decane, 2,3,5-tri...	10.73	2.6	ng	82881	4	11.33	632717	20.0
Trifluoroacetoxy ...	13.80	3.1	ng	93270	5	13.98	608538	20.0
9-Octadecenamide,...	14.73	7.0	ng	158276	6	15.45	454407	20.0
Supraene	14.82	5.5	ng	125160	6	15.45	454407	20.0