

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
 Data File : BF109280.D
 Acq On : 24 Sep 2018 20:48
 Operator : JU/SJ
 Sample : J5044-05
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GRID05-COMP-092018

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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	4.898	474	478	485	rBV	52677	63405	3.70%	0.393%
2	5.316	545	549	553	rBV	1607551	1558308	90.86%	9.651%
3	6.345	720	724	735	rVB	1715505	1715138	100.00%	10.622%
4	6.481	742	747	750	rBV	1899887	1649401	96.17%	10.215%
5	6.710	782	786	789	rBV	786361	588351	34.30%	3.644%
6	6.869	809	813	816	rBV	1507316	1303415	75.99%	8.072%
7	7.269	877	881	884	rBV	1209278	985643	57.47%	6.104%
8	7.992	1000	1004	1007	rBV	899341	716735	41.79%	4.439%
9	9.069	1183	1187	1190	rBV	2019596	1681599	98.04%	10.414%
10	9.457	1250	1253	1257	rBV	455072	378993	22.10%	2.347%
11	9.739	1298	1301	1305	rBV2	893118	733985	42.79%	4.546%
12	10.522	1431	1434	1442	rBV	1040726	931776	54.33%	5.771%
13	11.216	1549	1552	1555	rBV	799256	696410	40.60%	4.313%
14	11.239	1555	1556	1559	rVB	38875	24695	1.44%	0.153%
15	11.757	1640	1644	1648	rBV2	26902	33149	1.93%	0.205%
16	12.421	1755	1757	1761	rBV	52328	46545	2.71%	0.288%
17	12.651	1788	1796	1799	rBV	56653	65071	3.79%	0.403%
18	12.798	1817	1821	1825	rBV	1719084	1428623	83.29%	8.848%
19	13.280	1898	1903	1912	rBV	193605	224002	13.06%	1.387%
20	13.710	1973	1976	1983	rBV2	74610	116333	6.78%	0.720%
21	13.845	1995	1999	2002	rBV	711991	650321	37.92%	4.028%
22	14.627	2129	2132	2137	rVB	38917	43753	2.55%	0.271%
23	14.692	2141	2143	2146	rVV	55196	44791	2.61%	0.277%
24	15.245	2233	2237	2242	rBV	356904	415992	24.25%	2.576%
25	15.292	2243	2245	2251	rVB2	47337	50354	2.94%	0.312%

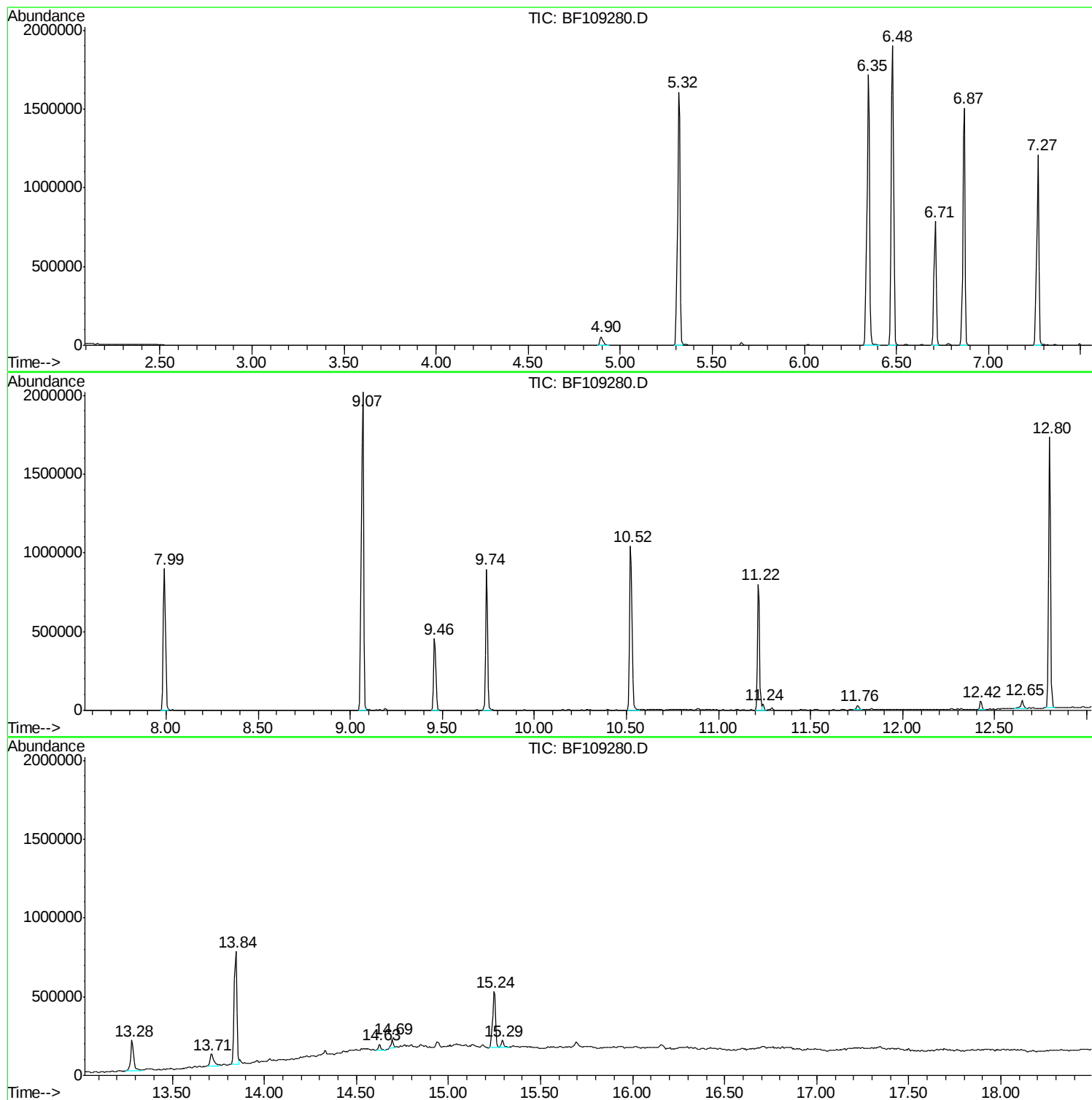
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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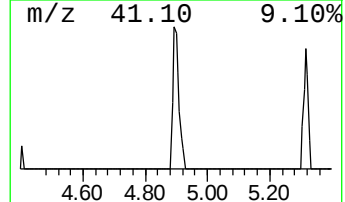
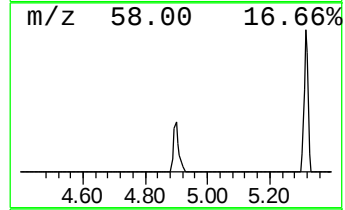
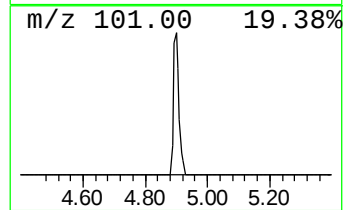
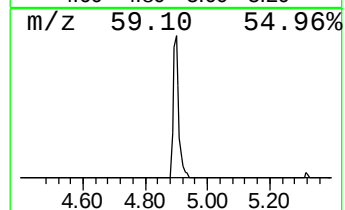
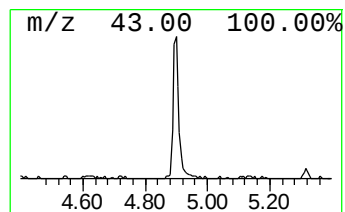
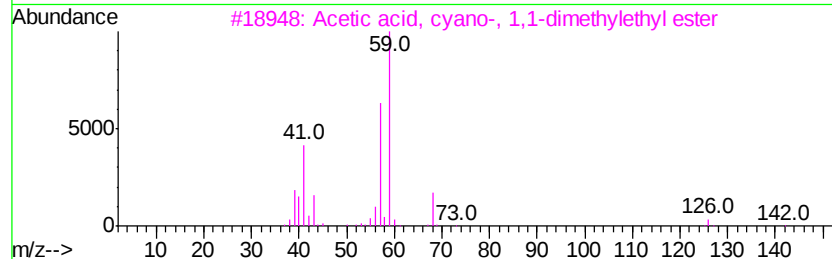
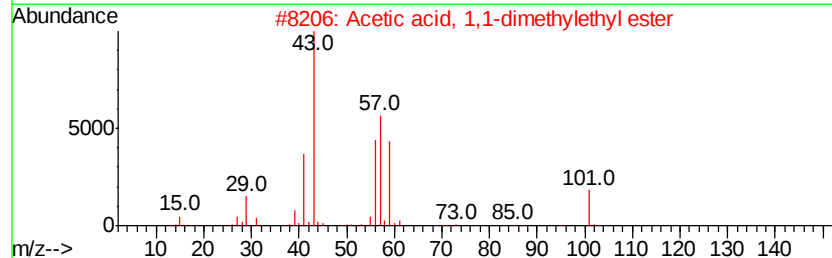
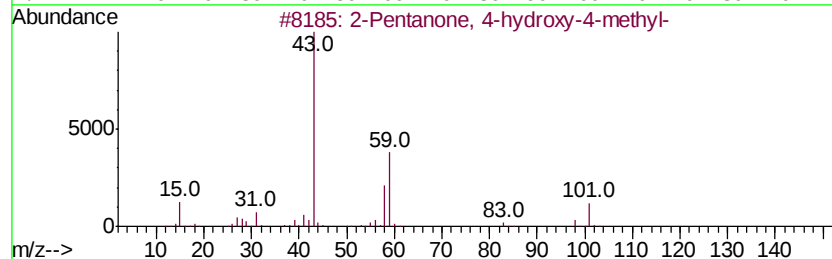
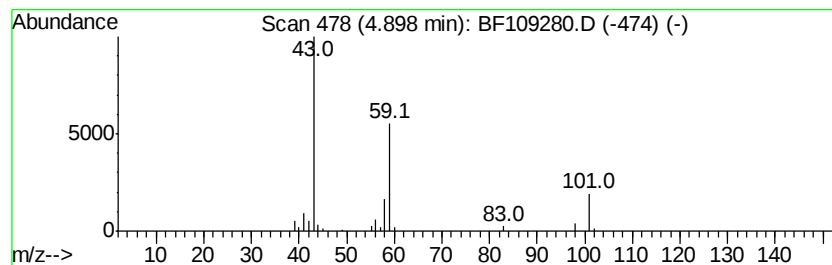
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.90	2.16 ng	63405	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5		Acetone	58	C3H6O	000067-64-1	9



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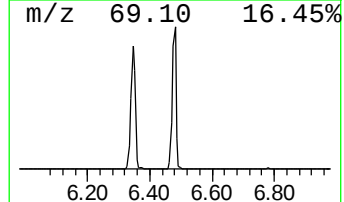
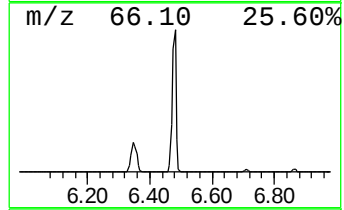
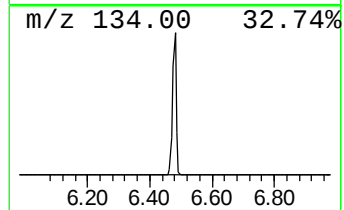
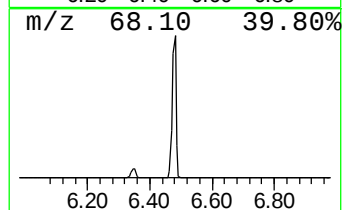
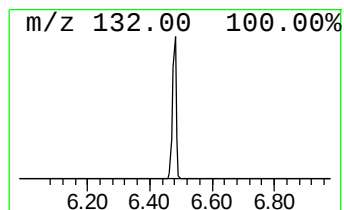
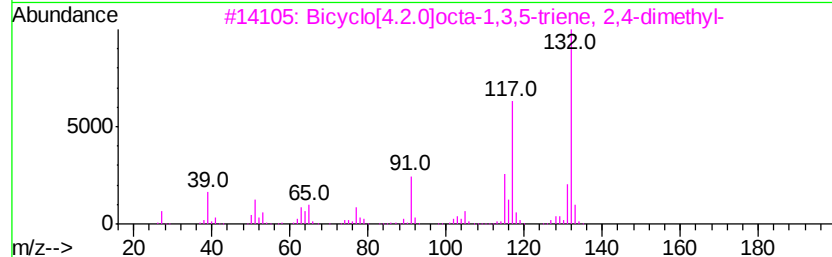
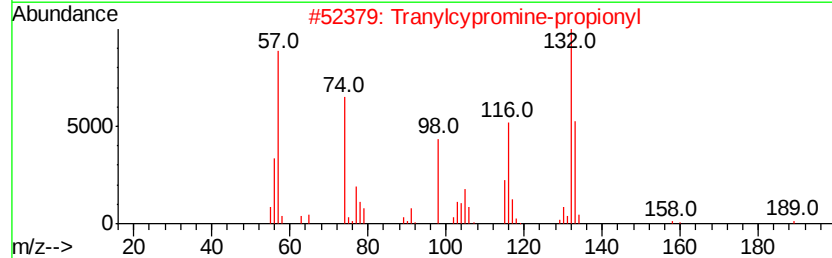
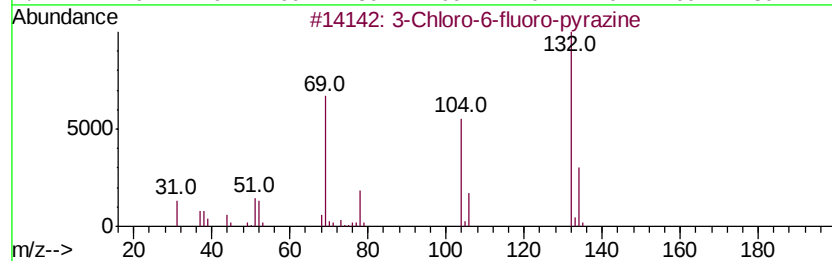
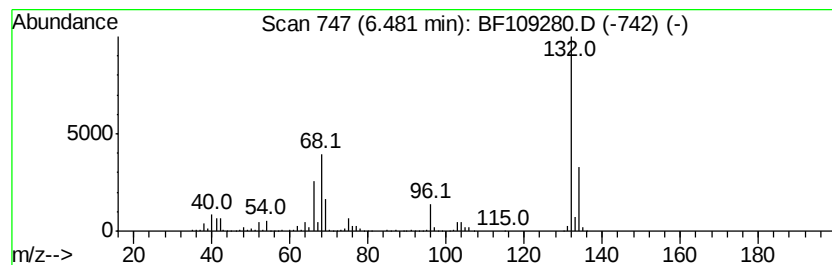
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	56.07 ng	1649400	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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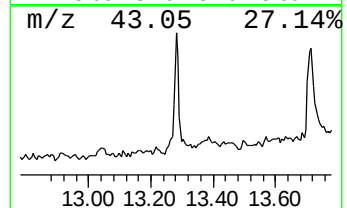
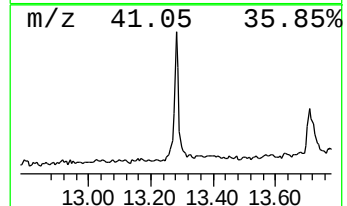
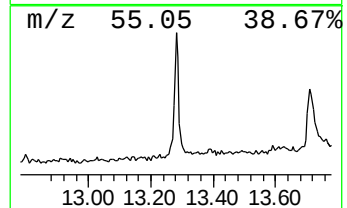
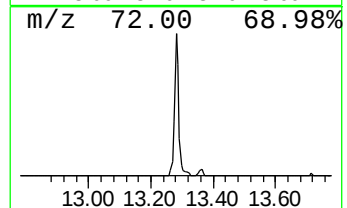
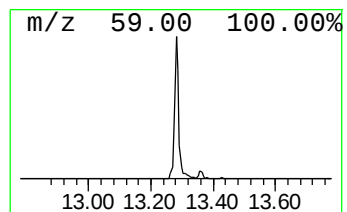
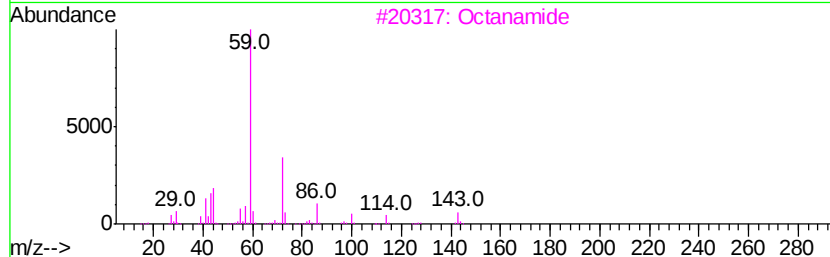
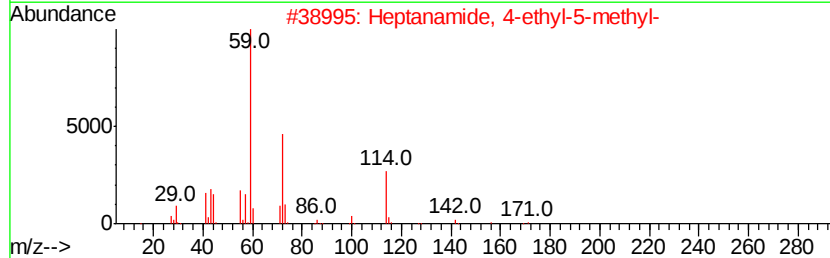
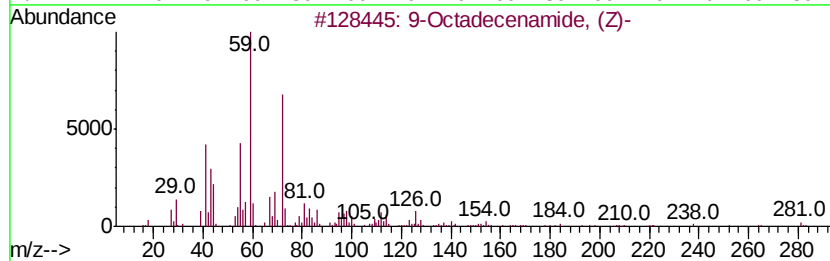
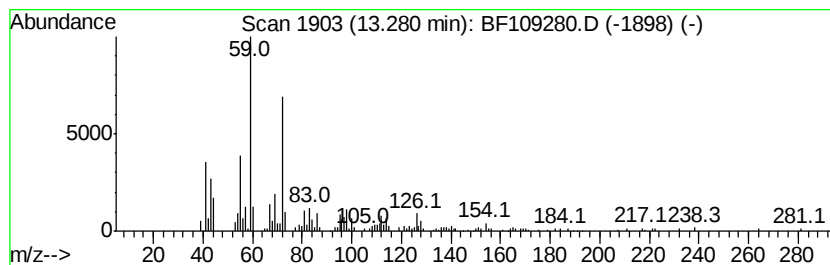
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TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.28	6.89 ng	224002	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3	Octanamide	143	C8H17NO	000629-01-6	59
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	43



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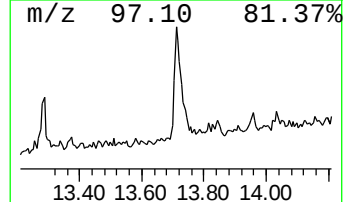
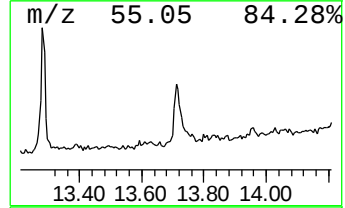
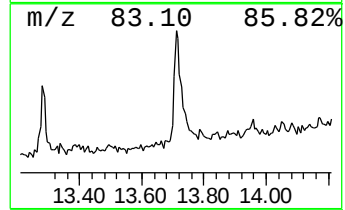
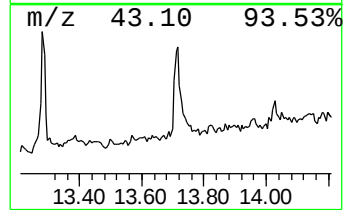
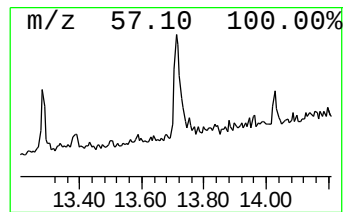
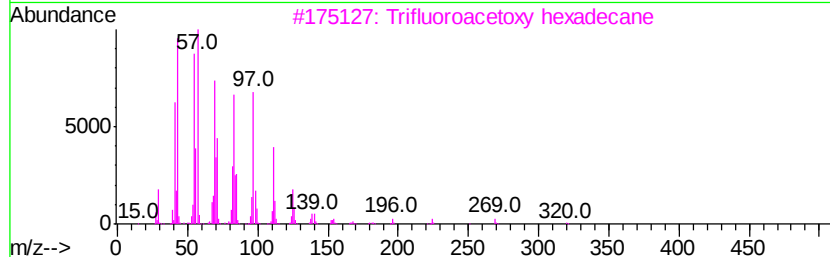
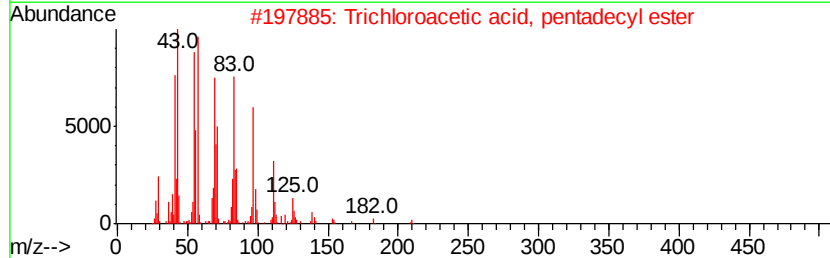
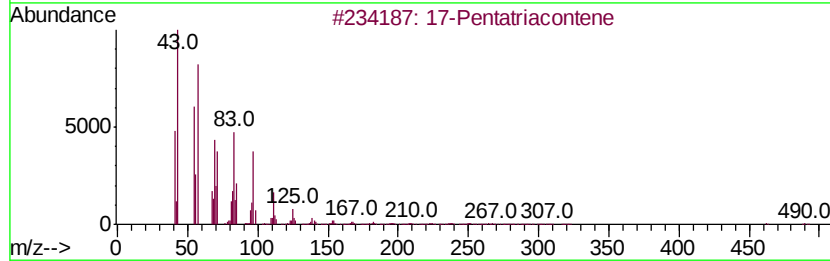
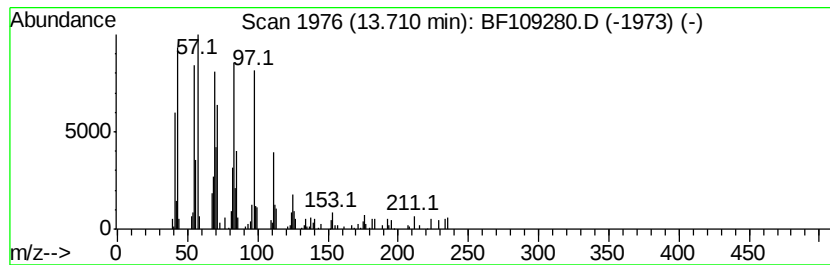
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 17-Pentatriacontene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.71	3.58 ng	116333	Chrysene-d12	13.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	91
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	74
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	64
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	62



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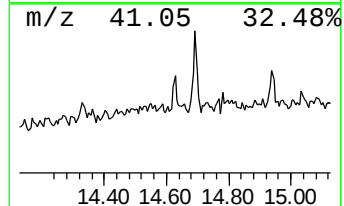
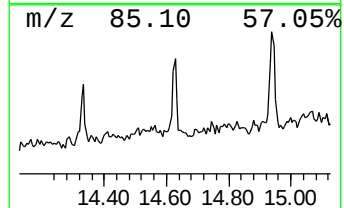
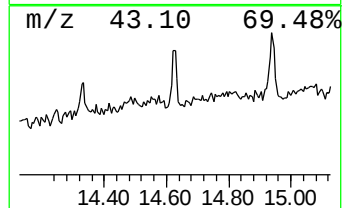
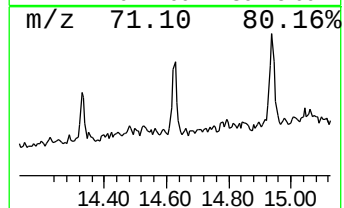
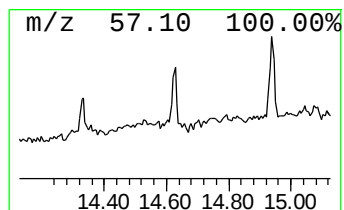
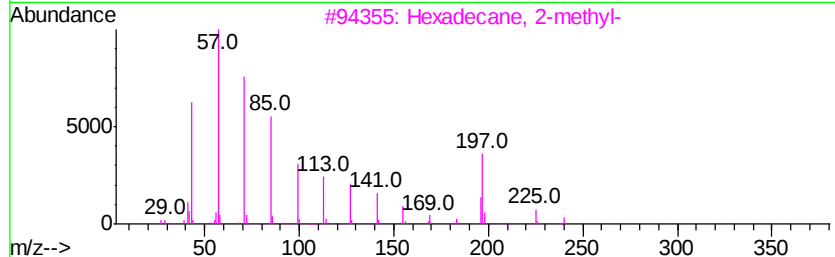
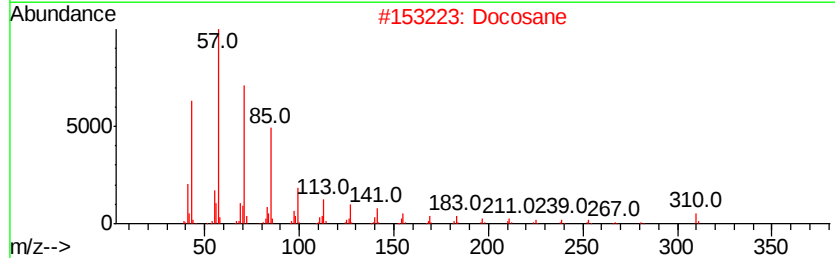
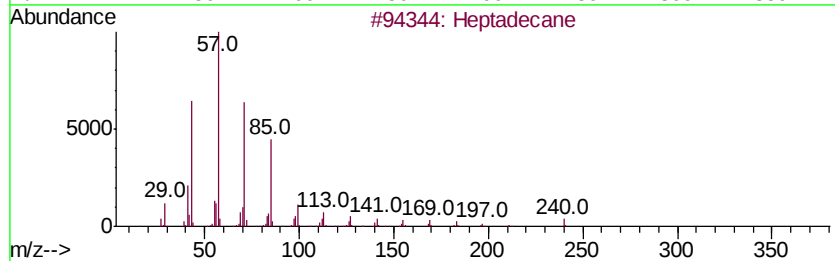
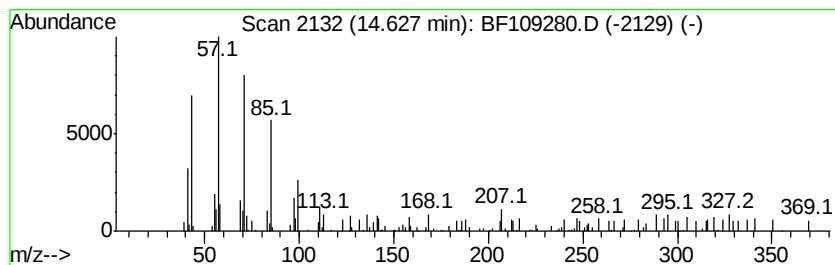
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.10 ng	43753	Perylene-d12	15.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	76
2	Docosane		310	C22H46	000629-97-0	74
3	Hexadecane, 2-methyl-		240	C17H36	001560-92-5	72
4	Heneicosane		296	C21H44	000629-94-7	72
5	Tricosane		324	C23H48	000638-67-5	72



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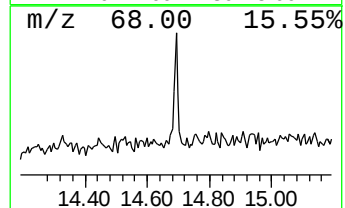
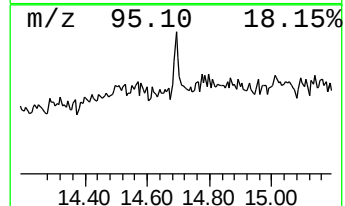
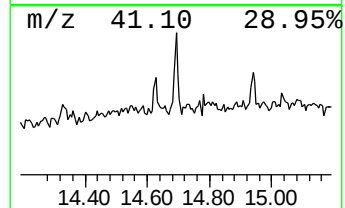
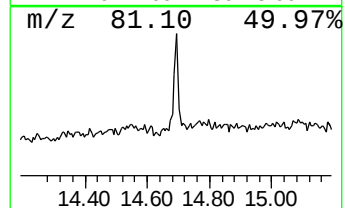
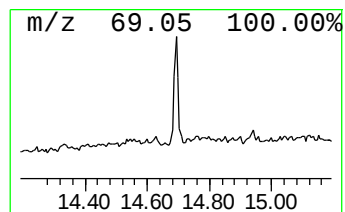
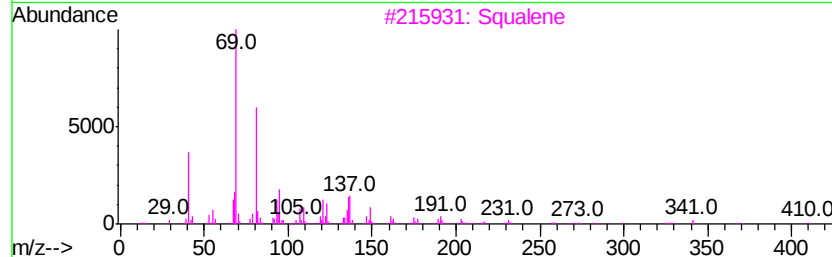
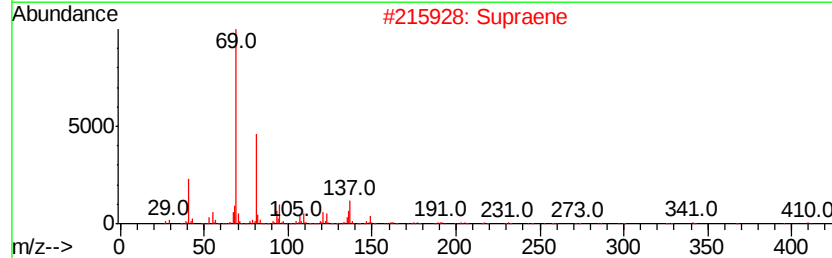
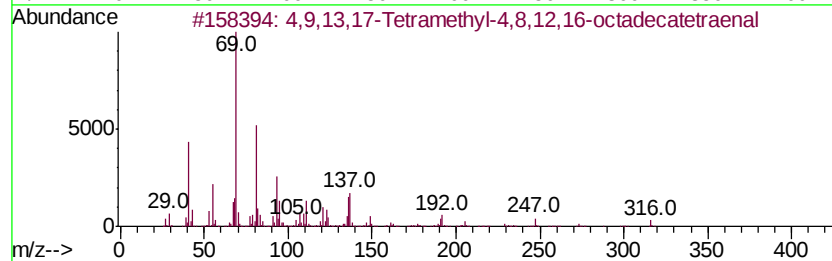
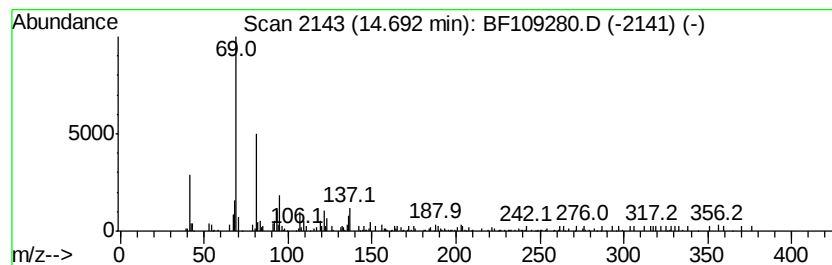
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 4,9,13,17-Tetramethyl-4,8,1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	2.15 ng	44791	Perylene-d12	15.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83		
2	Supraene	410	C30H50	007683-64-9	74		
3	Squalene	410	C30H50	000111-02-4	72		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72		
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64		



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092418\
Data File : BF109280.D
Acq On : 24 Sep 2018 20:48
Operator : JU/SJ
Sample : J5044-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GRID05-COMP-092018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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...	4.90	2.2	ng	63405	1	6.71	588351	20.0
unknown6.48	6.48	56.1	ng	1649400	1	6.71	588351	20.0
9-Octadecenamide, ...	13.28	6.9	ng	224002	5	13.84	650321	20.0
17-Pentatriacontene	13.71	3.6	ng	116333	5	13.84	650321	20.0
Heptadecane	14.63	2.1	ng	43753	6	15.24	415992	20.0
4,9,13,17-Tetrame...	14.69	2.1	ng	44791	6	15.24	415992	20.0