

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
 Data File : BF102277.D
 Acq On : 20 Jan 2018 20:22
 Operator : SJ/JU
 Sample : J1231-03
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-1A

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-BF010918.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	4.922	477	482	491	rBV	152872	207388	6.94%	0.759%
2	5.334	547	552	555	rBV	2913927	2824161	94.46%	10.340%
3	6.363	721	727	740	rBV	2792138	2989916	100.00%	10.947%
4	6.492	744	749	752	rBV	2945010	2893045	96.76%	10.592%
5	6.722	784	788	791	rBV	923454	817839	27.35%	2.994%
6	6.875	810	814	817	rBV	2613005	2197358	73.49%	8.045%
7	7.287	879	884	887	rBV	1908852	1748004	58.46%	6.400%
8	8.004	1001	1006	1009	rBV	1133767	1059117	35.42%	3.878%
9	8.557	1097	1100	1105	rBV	93325	80804	2.70%	0.296%
10	8.863	1149	1152	1158	rBV	32442	31518	1.05%	0.115%
11	8.963	1163	1169	1174	rBV2	31689	44781	1.50%	0.164%
12	9.081	1183	1189	1192	rBV	3165580	2925113	97.83%	10.710%
13	9.339	1226	1233	1239	rBV	195900	307336	10.28%	1.125%
14	9.445	1247	1251	1253	rBV	47270	44845	1.50%	0.164%
15	9.475	1253	1256	1262	rVB	398260	339583	11.36%	1.243%
16	9.686	1284	1292	1294	rBV	45641	43913	1.47%	0.161%
17	9.757	1299	1304	1307	rBV	1079116	1026840	34.34%	3.760%
18	10.186	1373	1377	1380	rBV	37800	36597	1.22%	0.134%
19	10.398	1410	1413	1419	rBV	177757	145826	4.88%	0.534%
20	10.469	1419	1425	1430	rVB	240077	209584	7.01%	0.767%
21	10.545	1431	1438	1441	rBV	1562595	1461827	48.89%	5.352%
22	10.657	1454	1457	1462	rBV2	37638	34678	1.16%	0.127%
23	11.239	1552	1556	1559	rBV	1009656	837492	28.01%	3.066%
24	12.821	1821	1825	1828	rBV	2142998	1888502	63.16%	6.914%
25	13.227	1890	1894	1897	rBV	152271	142962	4.78%	0.523%
26	13.510	1939	1942	1946	rVB2	36301	33625	1.12%	0.123%
27	13.586	1952	1955	1960	rBV	216702	173418	5.80%	0.635%
28	13.716	1973	1977	1983	rBV	315213	328659	10.99%	1.203%
29	13.874	2000	2004	2007	rBV	780594	719293	24.06%	2.634%
30	13.974	2013	2021	2030	rVB7	86384	289508	9.68%	1.060%
31	14.274	2069	2072	2076	rBV	320417	276624	9.25%	1.013%
32	14.351	2082	2085	2091	rVB2	125751	129783	4.34%	0.475%
33	14.451	2100	2102	2108	rVB5	35636	39257	1.31%	0.144%
34	14.639	2132	2134	2138	rBV4	27249	38932	1.30%	0.143%

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Stop Thrs : 0 Peak Location: TOP

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35	14.686	2138	2142	2145	rBV	158080	166501	5.57%	0.610%
36	14.963	2186	2189	2191	rBV3	40441	44394	1.48%	0.163%
37	15.298	2240	2246	2253	rBV	482110	675756	22.60%	2.474%
38	15.727	2316	2319	2324	rVB3	47094	57905	1.94%	0.212%

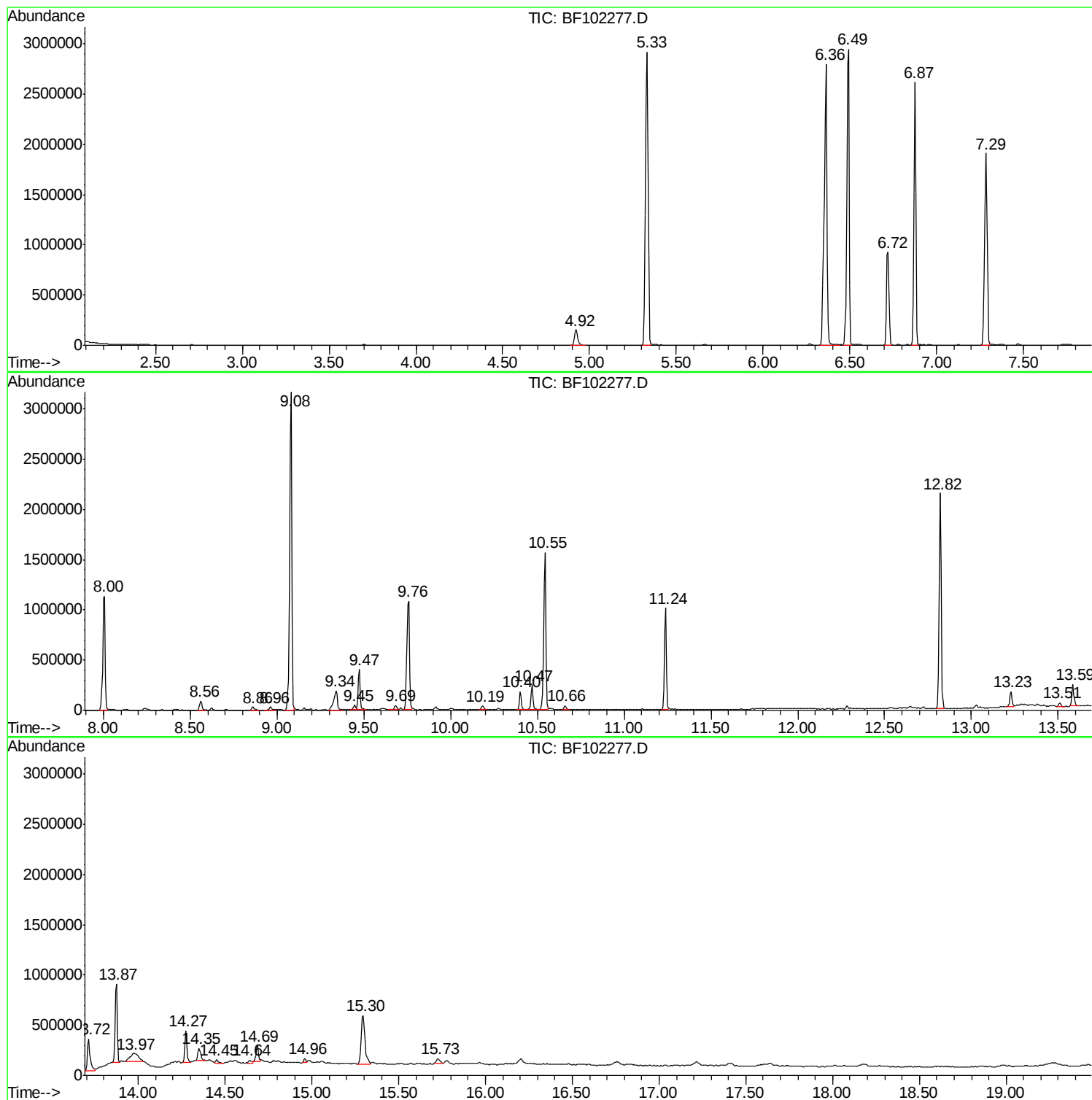
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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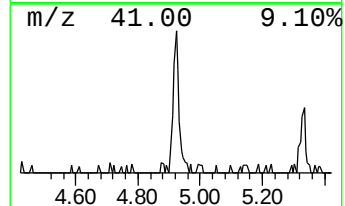
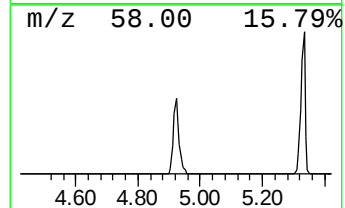
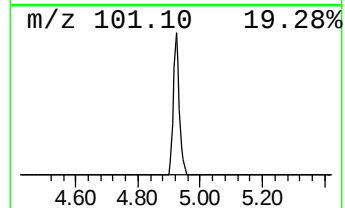
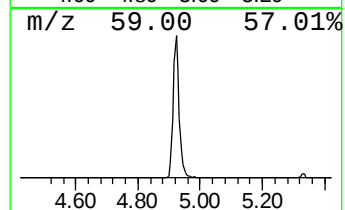
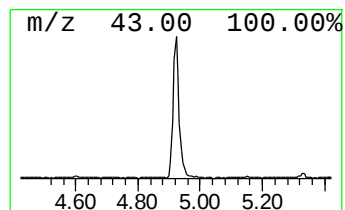
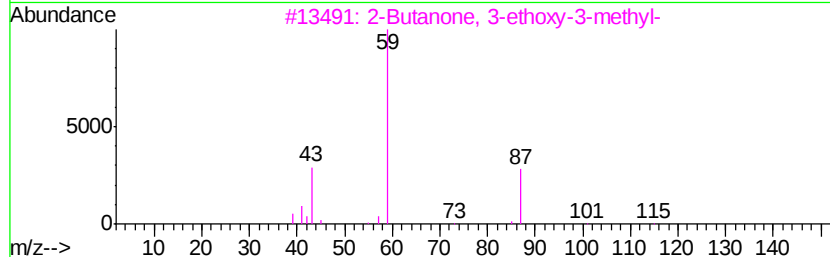
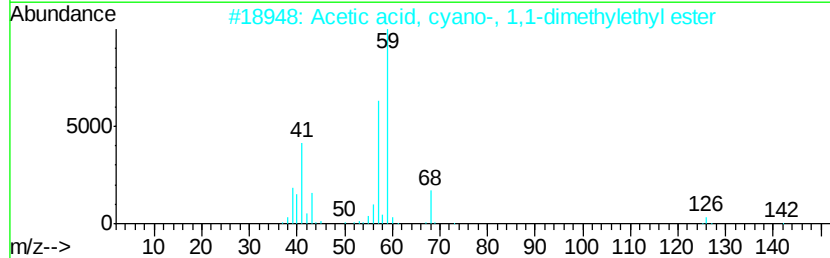
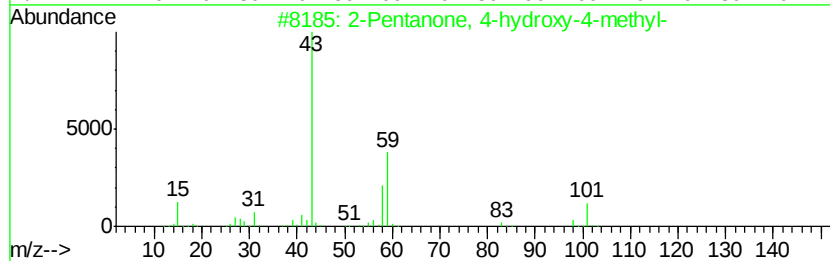
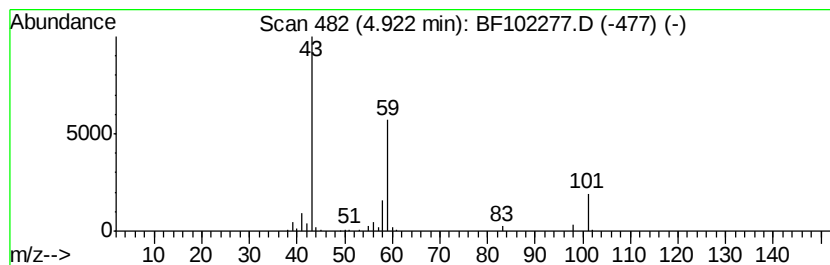
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.07 ng	207388	1,4-Dichlorobenzene-d4	6.72

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	9
3		2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5		3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9



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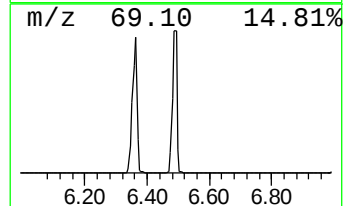
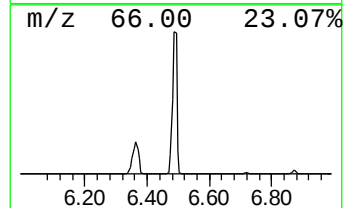
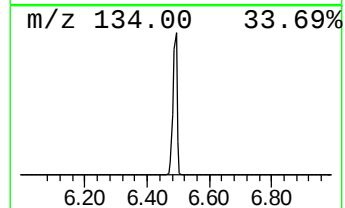
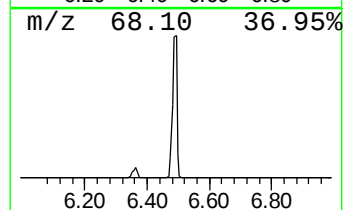
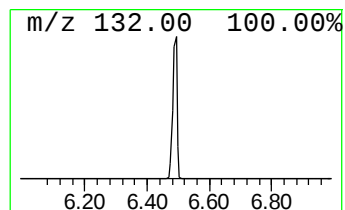
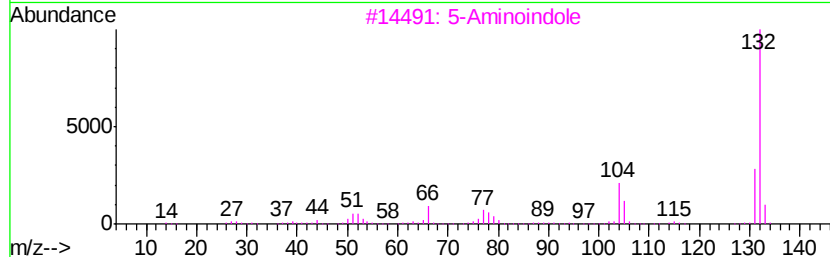
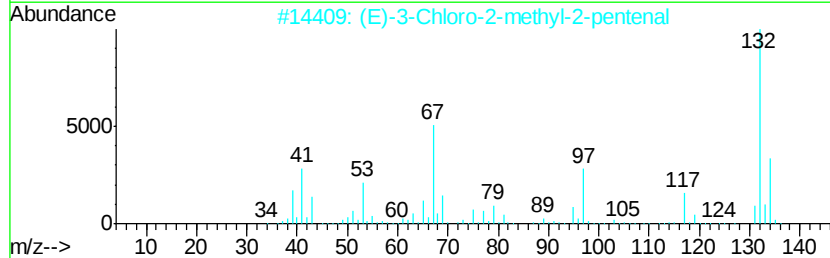
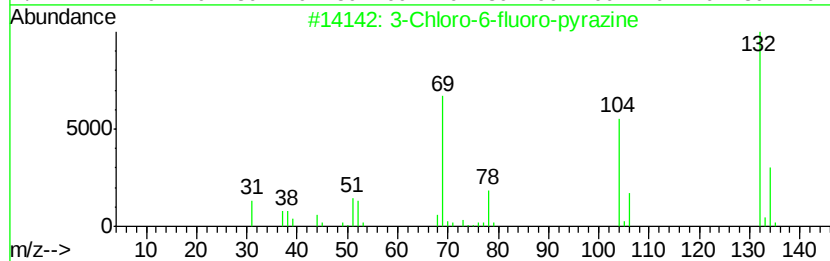
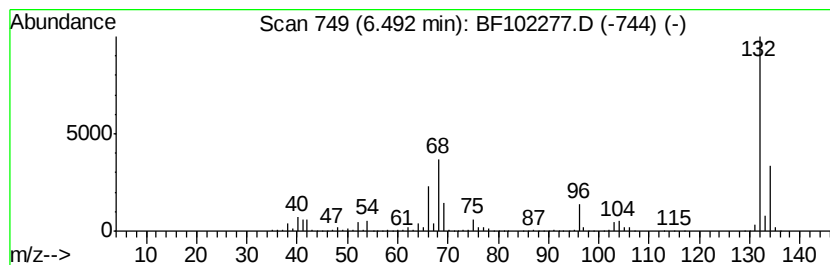
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	70.75 ng	2893050	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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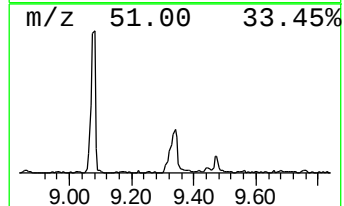
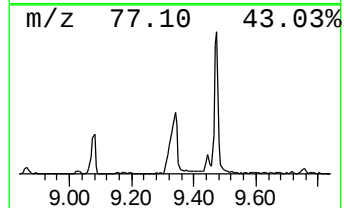
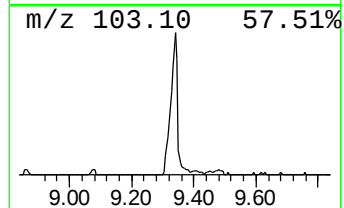
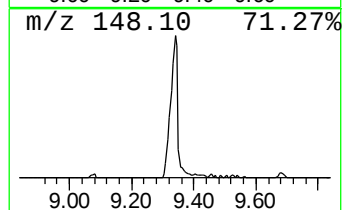
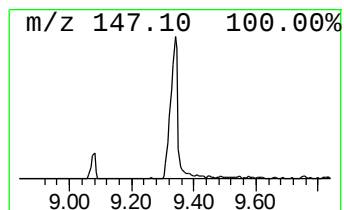
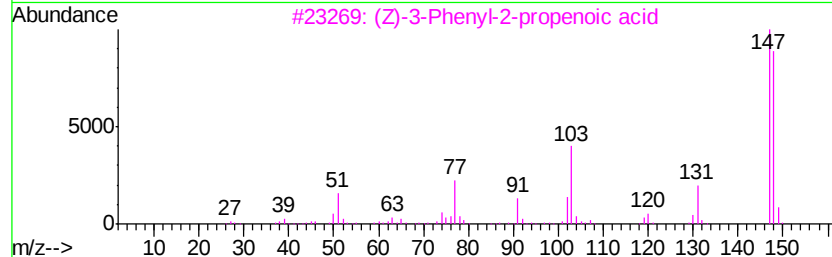
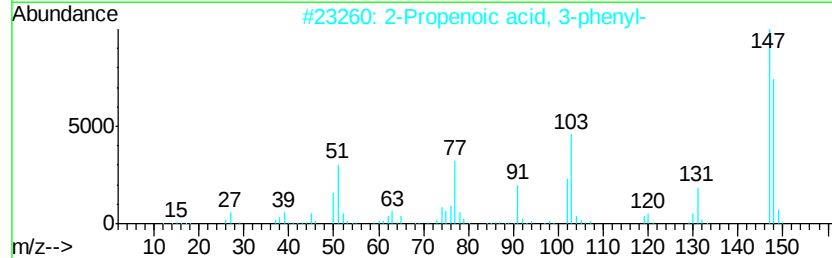
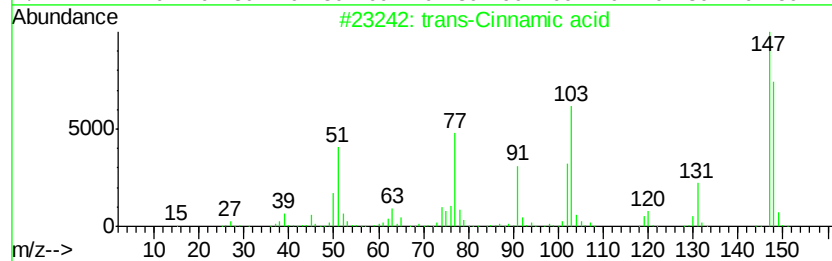
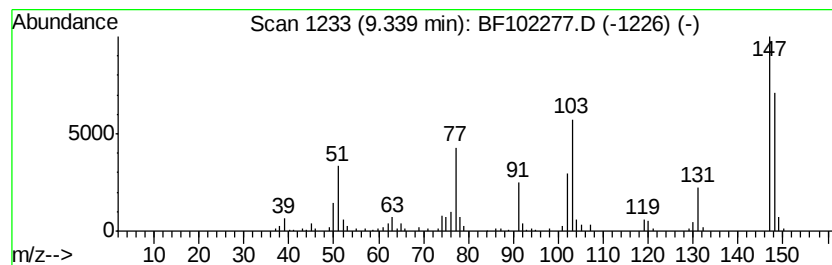
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 trans-Cinnamic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.34	5.99 ng	307336	Acenaphthene-d10	9.76

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Cinnamic acid	148	C9H8O2	000140-10-3	98
2			2-Propenoic acid, 3-phenyl-	148	C9H8O2	000621-82-9	98
3			(Z)-3-Phenyl-2-propenoic acid	148	C9H8O2	000102-94-3	94
4			Bicyclo[4.2.0]octa-1,3,5-triene...	148	C9H8O2	014381-41-0	52
5			4-Vinylbenzoic acid	148	C9H8O2	001075-49-6	43



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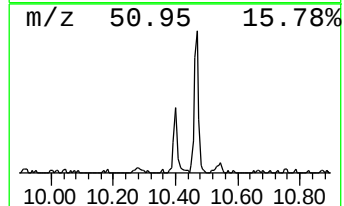
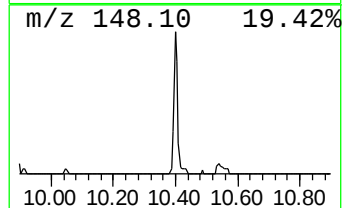
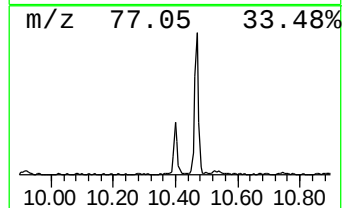
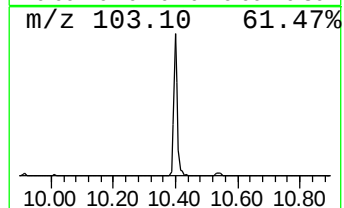
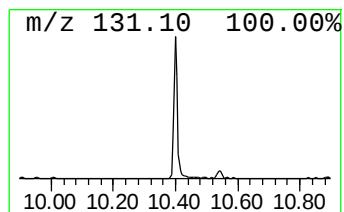
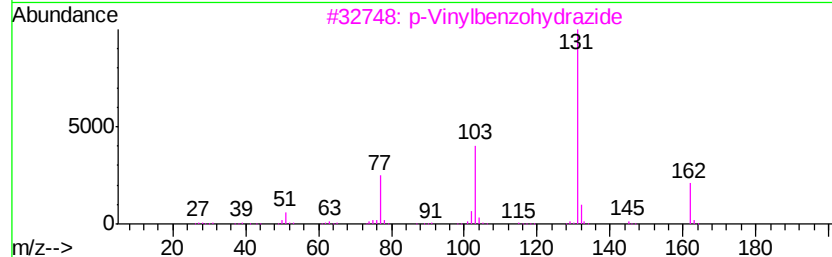
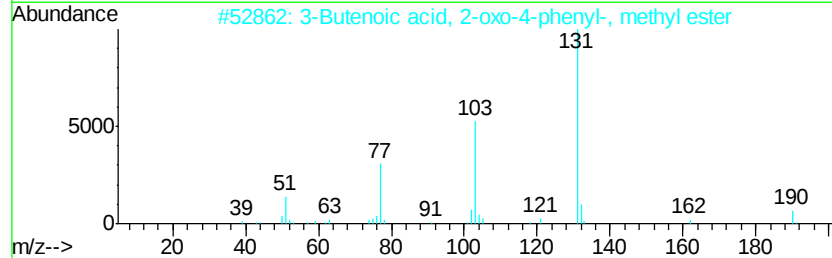
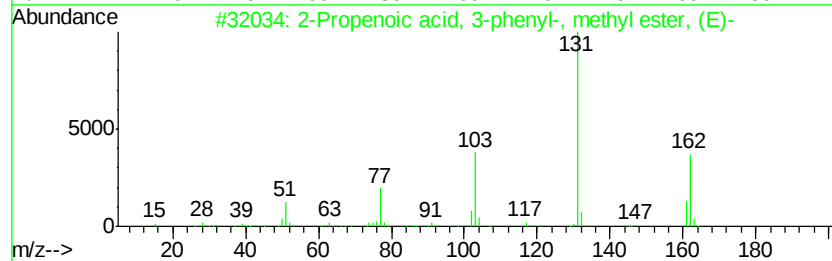
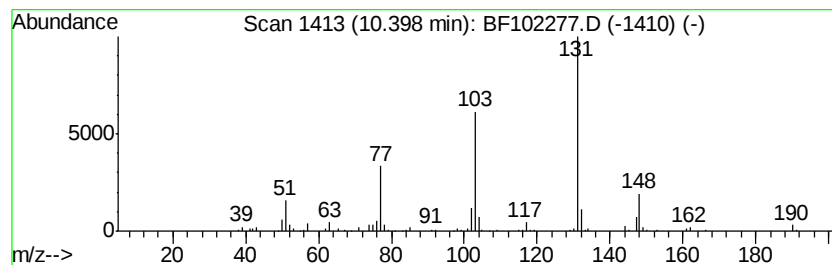
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Peak Number 5 2-Propenoic acid, 3-phenyl-... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.40	2.84 ng	145826	Acenaphthene-d10	9.76

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	87
2		3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	87
3		p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	83
4		2-Propenyl chloride, 3-phenyl-,...	166	C9H7ClO	017082-09-6	83
5		Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	72



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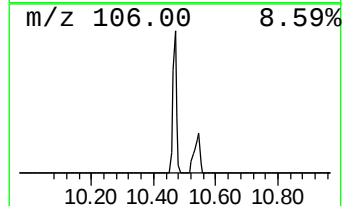
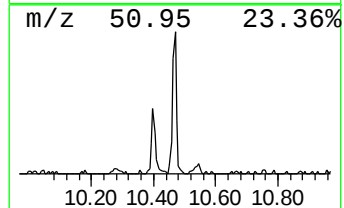
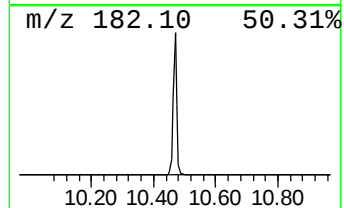
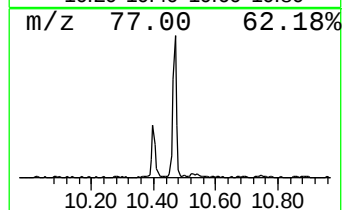
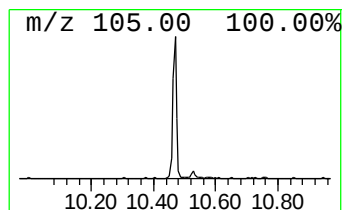
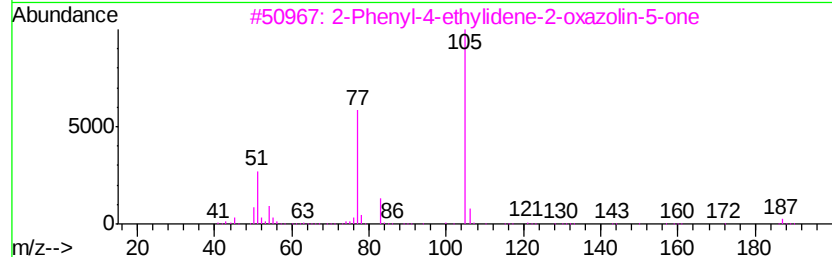
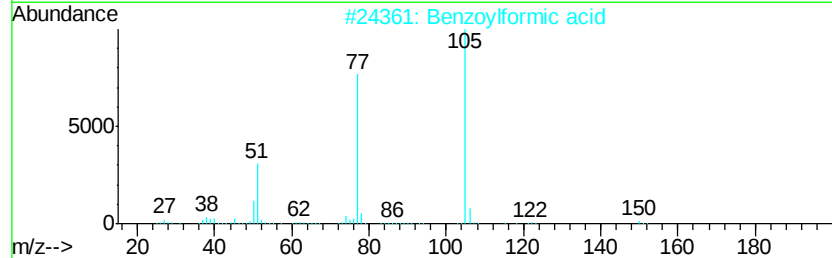
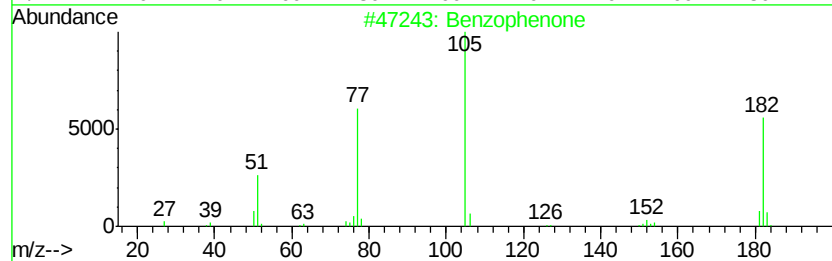
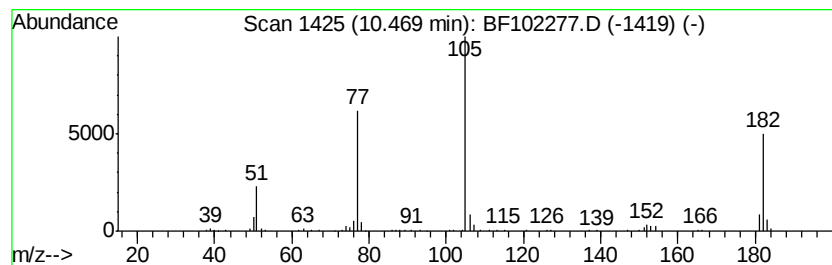
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Peak Number 6 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.47	4.08 ng	209584	Acenaphthene-d10	9.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoylformic acid	150	C8H6O3	000611-73-4	47
3	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Vinyl benzoate	148	C9H8O2	000769-78-8	47



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
Data File : BF102277.D
Acq On : 20 Jan 2018 20:22
Operator : SJ/JU
Sample : J1231-03
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-1A

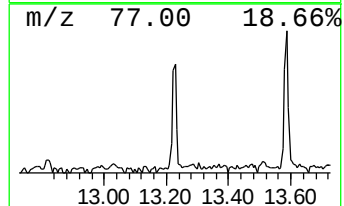
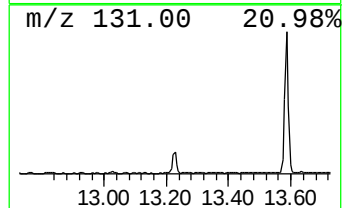
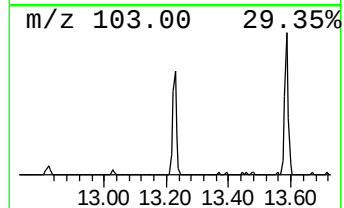
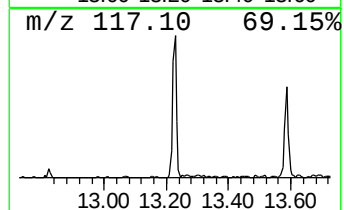
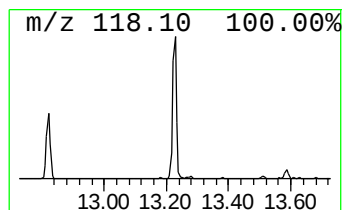
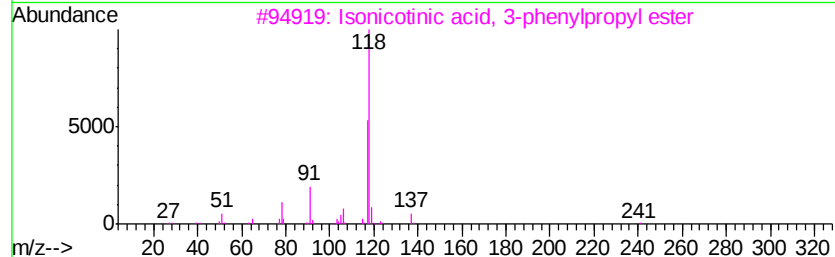
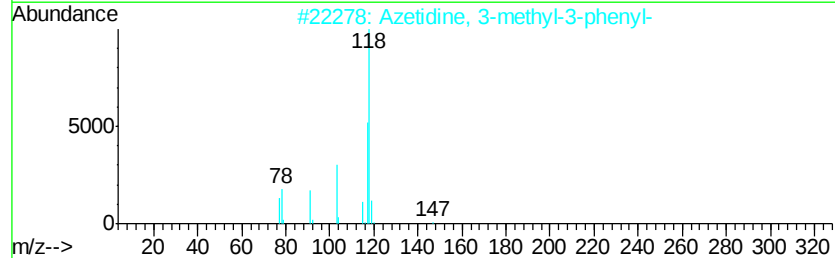
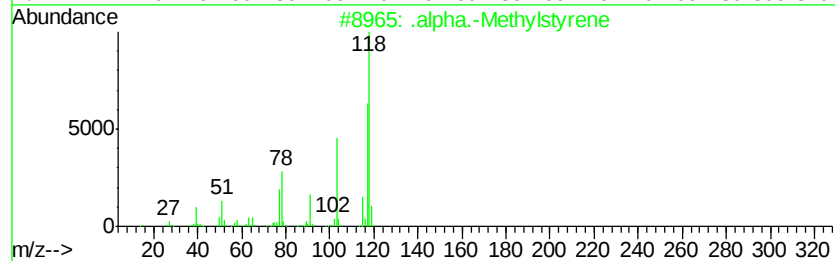
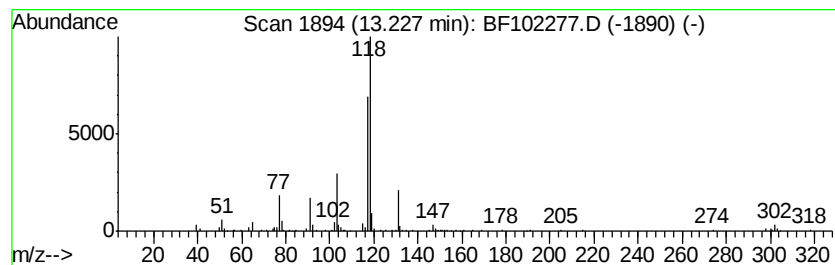
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 .alpha.-Methylstyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.23	3.98 ng	142962	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Methylstvrene	118	C9H10	000098-83-9	64
2		Azetidine, 3-methyl-3-phenyl-	147	C10H13N	005961-33-1	59
3		Isonicotinic acid, 3-phenylpropyl...	241	C15H15NO2	1000308-36-4	53
4		3-Phenyl-1-propanol, acetate	178	C11H14O2	000122-72-5	53
5		Pentanoic acid, 3-phenylpropyl e...	220	C14H20O2	005451-88-7	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
Data File : BF102277.D
Acq On : 20 Jan 2018 20:22
Operator : SJ/JU
Sample : J1231-03
Misc :
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ClientSampleId :
RW-1A

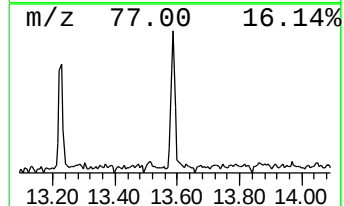
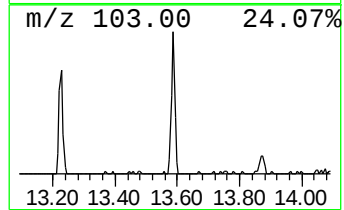
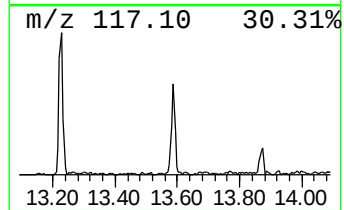
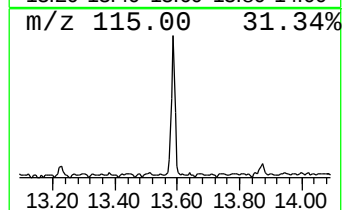
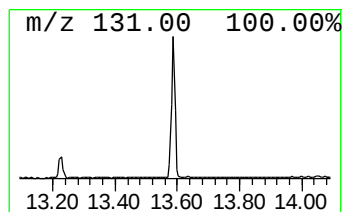
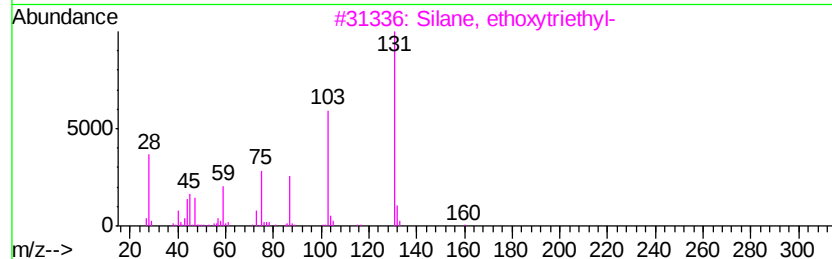
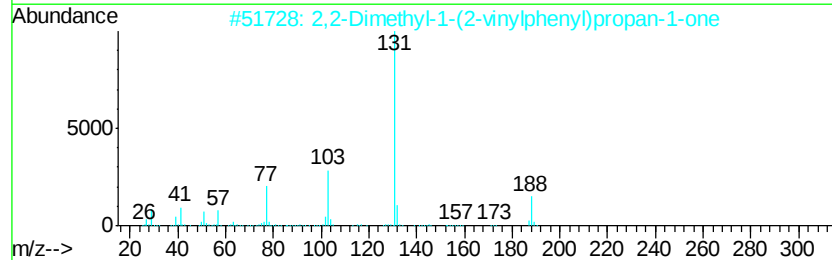
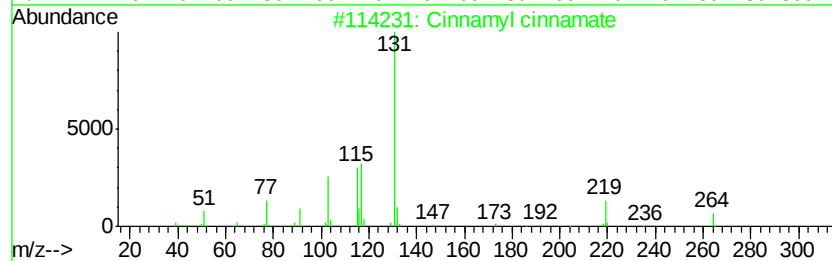
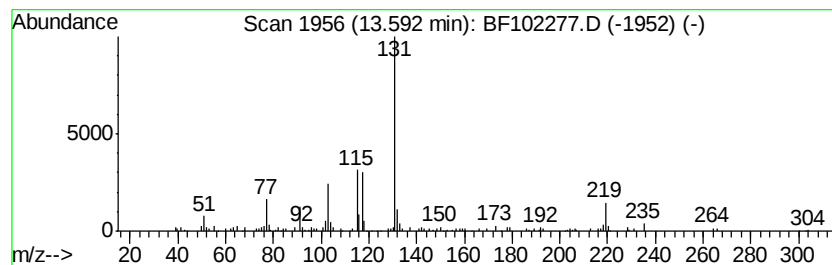
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cinnamyl cinnamate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	4.82 ng	173418	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91	
2	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	52	
3	Silane, ethoxvtriethyl-	160	C8H20OSi	000597-67-1	50	
4	1-Penten-3-one, 4,4-dimethyl-1-p...	188	C13H16O	000538-44-3	50	
5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	50	



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\
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Sample : J1231-03
Misc :
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ClientSampleId :
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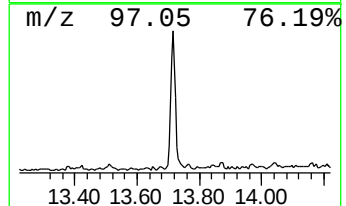
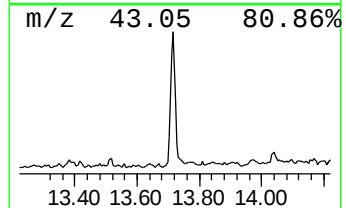
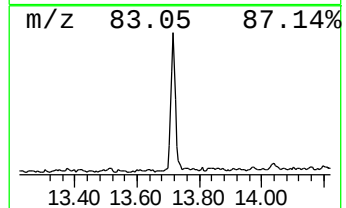
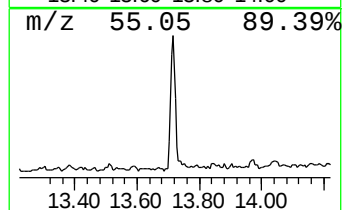
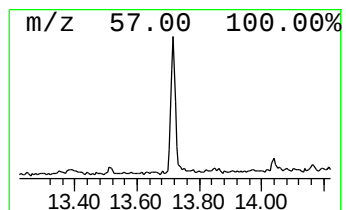
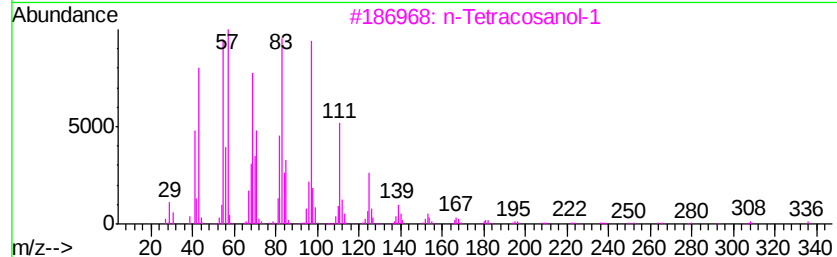
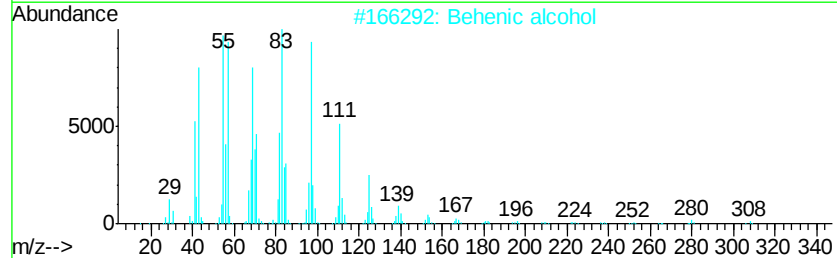
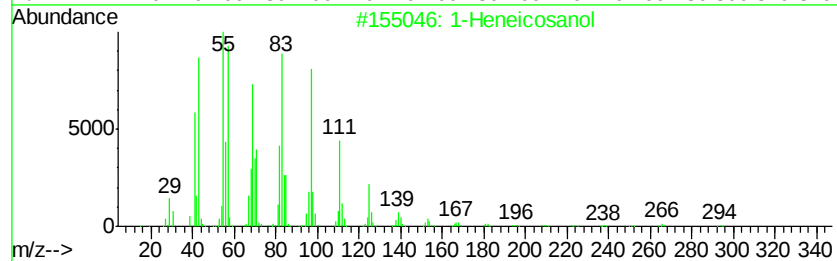
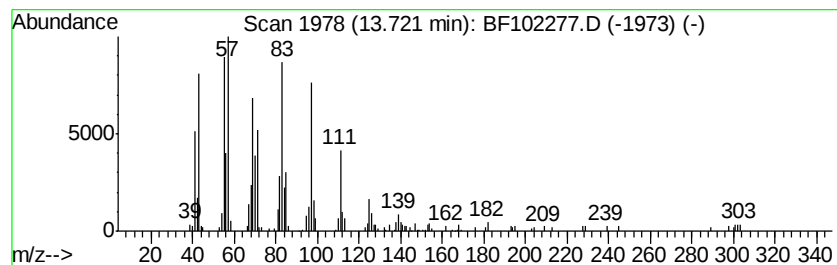
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	9.14 ng	328659	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Behenic alcohol	326	C22H46O	000661-19-8	95
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
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Acq On : 20 Jan 2018 20:22
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Misc :
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ClientSampleId :
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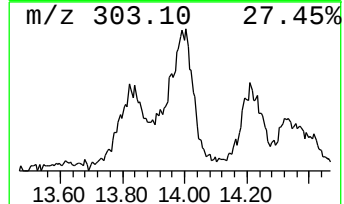
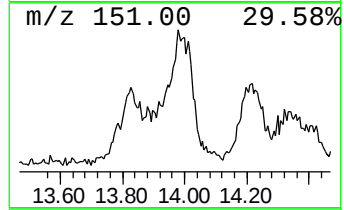
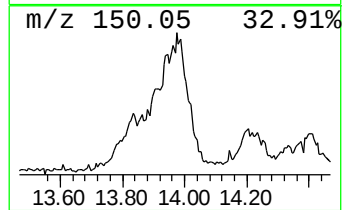
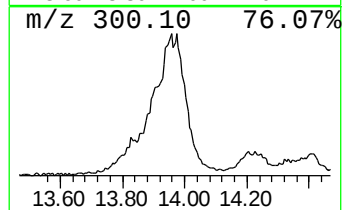
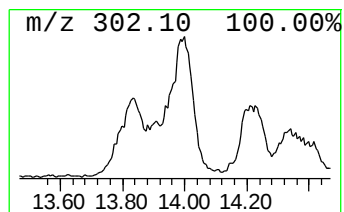
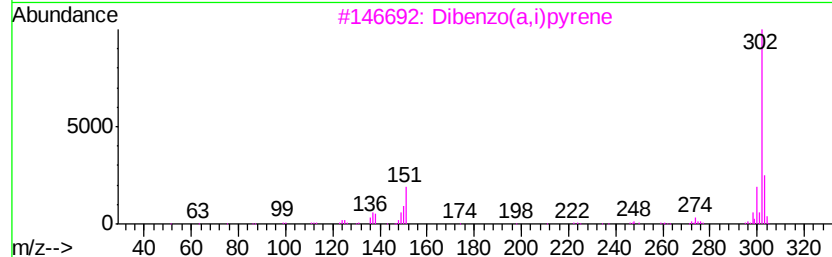
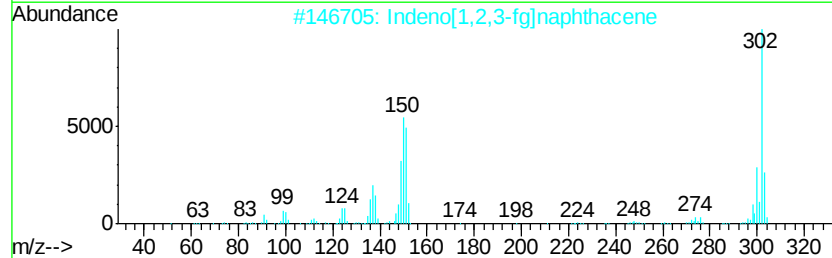
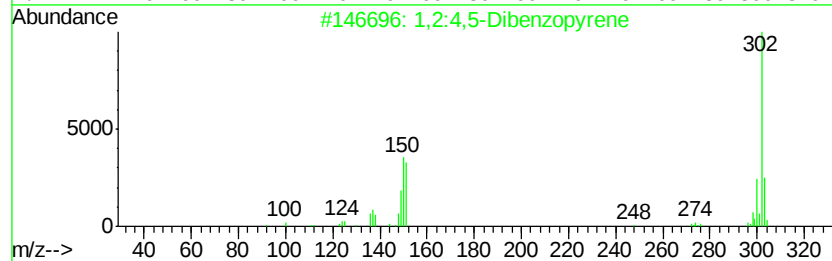
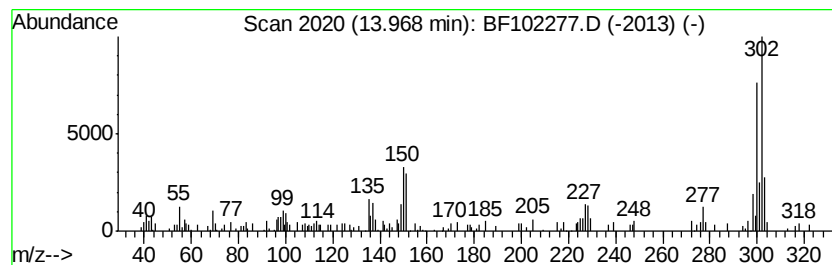
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,2:4,5-Dibenzopyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	8.05 ng	289508	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2:4,5-Dibenzopyrene	302	C24H14	000192-65-4	92
2			Indeno[1,2,3-fg]naphthacene	302	C24H14	000203-11-2	70
3			Dibenzo(a,i)pyrene	302	C24H14	000189-55-9	64
4			3,4:8,9-Dibenzopyrene	302	C24H14	000189-64-0	60
5			Dibenz(a,e)aceanthrylene	302	C24H14	005385-75-1	53



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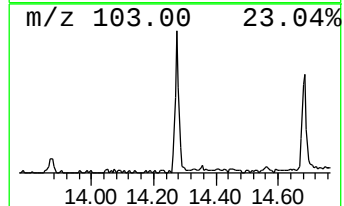
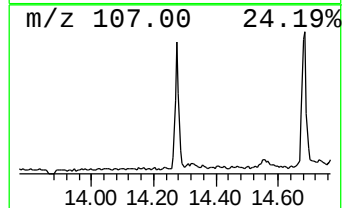
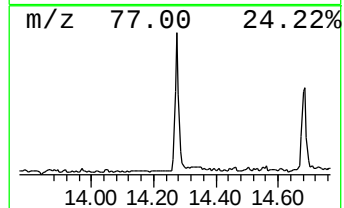
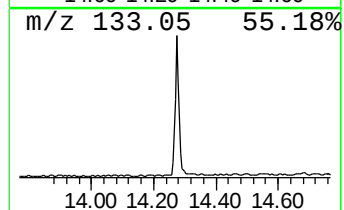
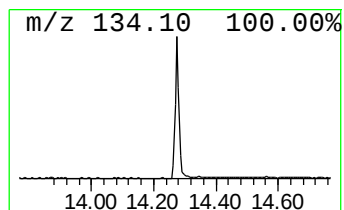
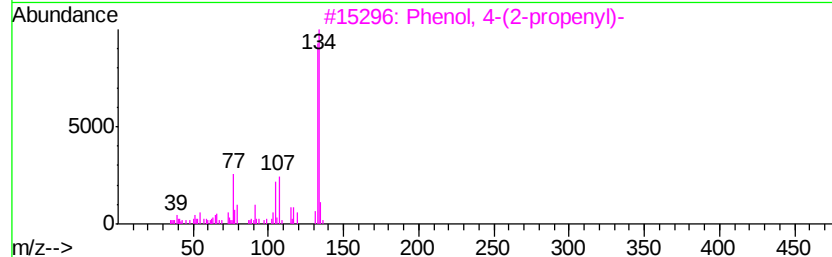
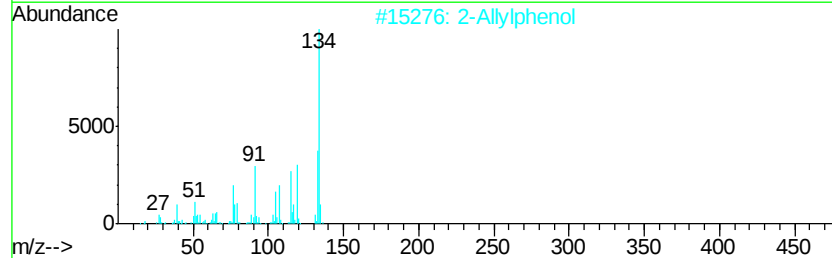
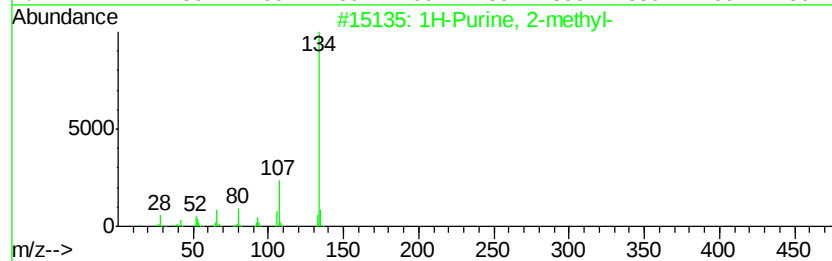
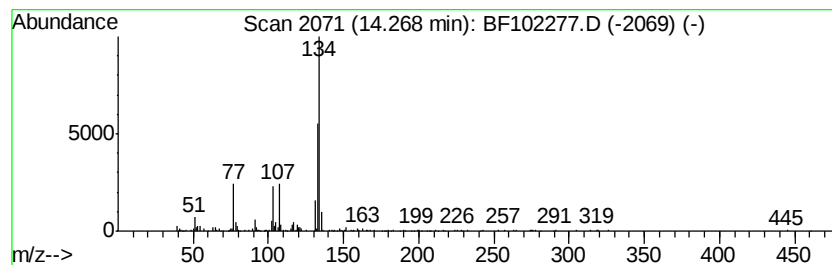
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown14.27 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	7.69 ng	276624	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Purine, 2-methyl-	134	C6H6N4	000934-23-6	43
2		2-Allylphenol	134	C9H10O	001745-81-9	42
3		Phenol, 4-(2-propenyl)-	134	C9H10O	000501-92-8	40
4		5,6,7,8-Tetrahydroquinoxaline	134	C8H10N2	034413-35-9	40
5		Tricyclo[4.2.2.2(2,5)]dodecan-3-one	178	C12H18O	068177-17-3	38



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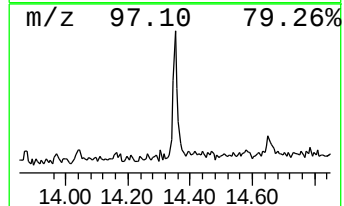
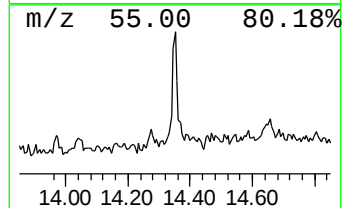
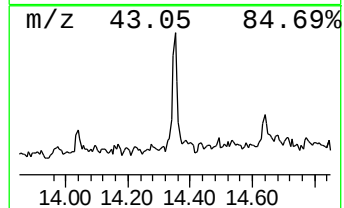
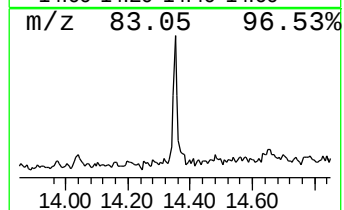
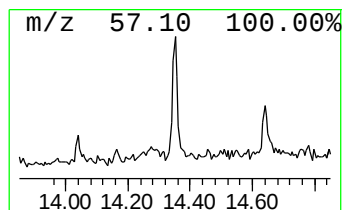
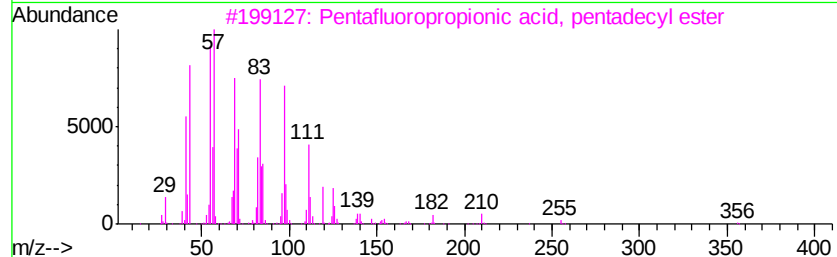
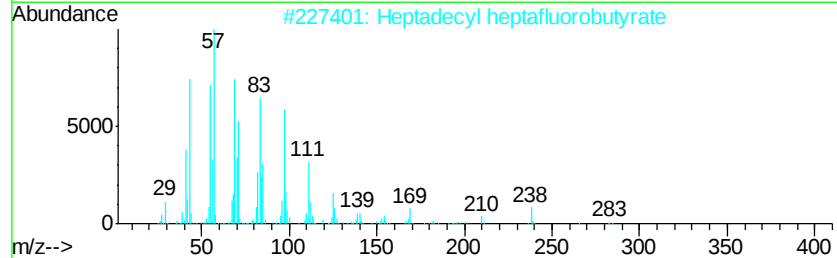
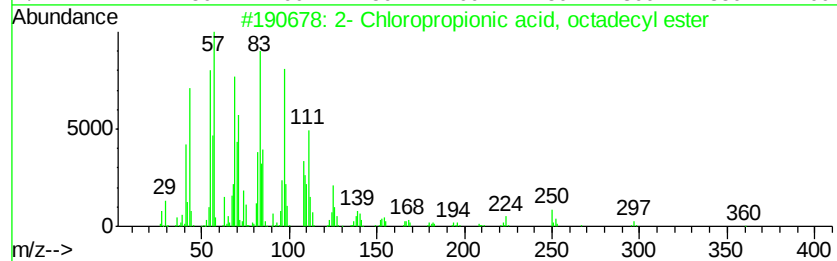
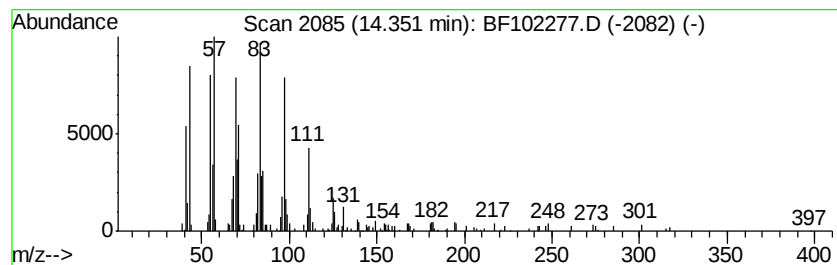
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2- Chloropropionic acid, oc... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.61 ng	129783	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



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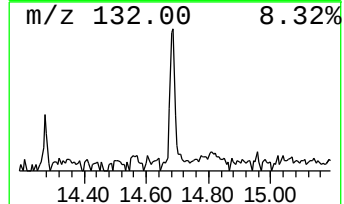
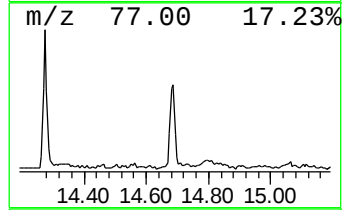
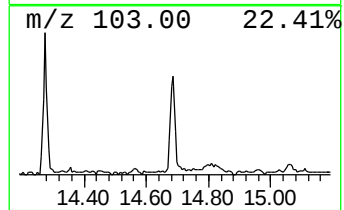
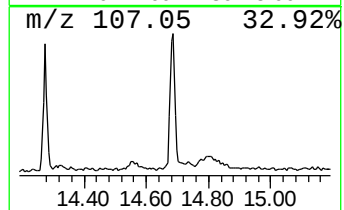
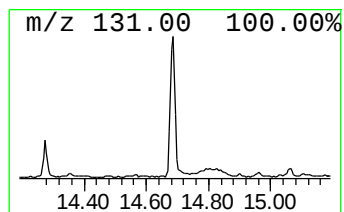
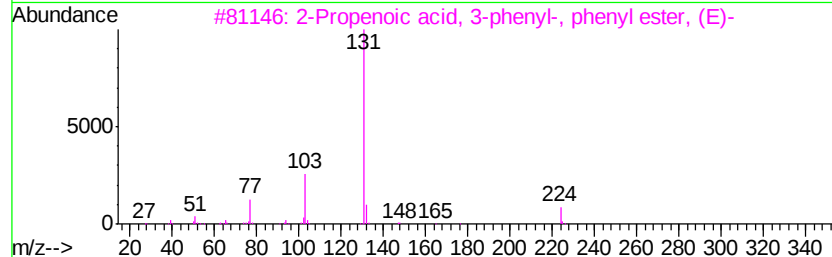
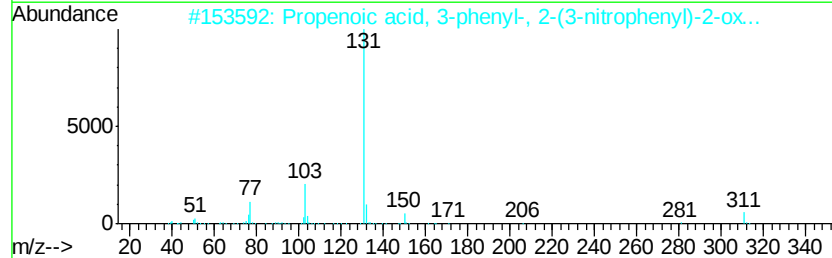
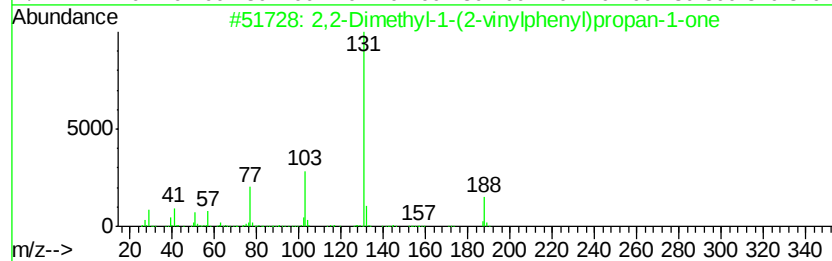
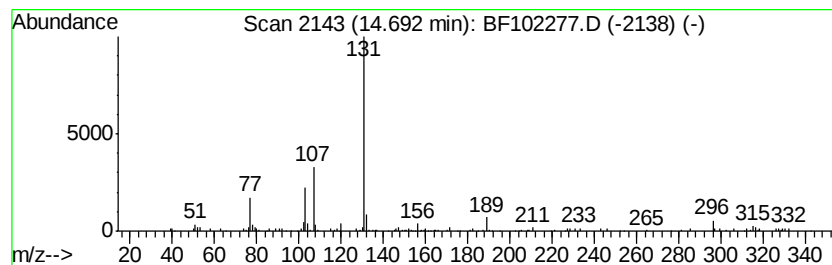
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2,2-Dimethyl-1-(2-vinylphen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.93 ng	166501	Perylene-d12	15.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	53
2		Propenoic acid, 3-phenyl-, 2-(3-...	311	C17H13NO5	1000264-14-5	50
3		2-Propenoic acid, 3-phenyl-, phe...	224	C15H12O2	025695-77-6	50
4		2-Propenamide, N-(4-bromophenyl)...	301	C15H12BrNO	054934-81-5	50
5		4-Pentenoic acid, 2,2-diethyl-3-...	274	C17H22O3	337503-48-7	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012018\
 Data File : BF102277.D
 Acq On : 20 Jan 2018 20:22
 Operator : SJ/JU
 Sample : J1231-03
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-1A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.92	5.1 ng		207388	1	6.72	817839	20.0
unknown6.49	6.49	70.8 ng		2893050	1	6.72	817839	20.0
trans-Cinnamic acid	9.34	6.0 ng		307336	3	9.76	1026840	20.0
2-Propenoic acid,...	10.40	2.8 ng		145826	3	9.76	1026840	20.0
Benzophenone	10.47	4.1 ng		209584	3	9.76	1026840	20.0
.alpha.-Methylsty...	13.23	4.0 ng		142962	5	13.87	719293	20.0
Cinnamyl cinnamate	13.59	4.8 ng		173418	5	13.87	719293	20.0
1-Heneicosanol	13.72	9.1 ng		328659	5	13.87	719293	20.0
1,2:4,5-Dibenzopy...	13.97	8.1 ng		289508	5	13.87	719293	20.0
unknown14.27	14.27	7.7 ng		276624	5	13.87	719293	20.0
2- Chloropropioni...	14.35	3.6 ng		129783	5	13.87	719293	20.0
2,2-Dimethyl-1-(2...	14.69	4.9 ng		166501	6	15.30	675756	20.0