

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096577.D
 Acq On : 7 Jul 2017 23:40
 Operator : SJ/MA
 Sample : I4070-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AU-05-070517-D

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-BF070117.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	4.887	470	476	487	rVB	353840	481900	17.47%	1.949%
2	5.310	543	548	551	rBV	2718610	2705211	98.09%	10.942%
3	6.340	717	723	740	rVB	2441659	2757872	100.00%	11.155%
4	6.469	740	745	748	rBV	2603431	2656281	96.32%	10.744%
5	6.692	780	783	787	rBV	813573	687362	24.92%	2.780%
6	6.851	806	810	813	rBV	2231991	1973320	71.55%	7.982%
7	7.257	873	879	882	rBV	1851486	1703987	61.79%	6.892%
8	7.975	997	1001	1005	rBV	1082455	924306	33.52%	3.739%
9	9.057	1180	1185	1188	rBV	2621422	2534155	91.89%	10.250%
10	9.145	1194	1200	1204	rBV4	31657	36973	1.34%	0.150%
11	9.445	1248	1251	1254	rBV	281347	214501	7.78%	0.868%
12	9.633	1277	1283	1287	rBV3	21830	43787	1.59%	0.177%
13	9.675	1287	1290	1293	rVB	50127	39317	1.43%	0.159%
14	9.728	1293	1299	1303	rBV	1086967	940122	34.09%	3.803%
15	10.145	1364	1370	1372	rBV3	24773	33690	1.22%	0.136%
16	10.175	1372	1375	1378	rVB	71553	57370	2.08%	0.232%
17	10.392	1407	1412	1415	rBV	26683	35219	1.28%	0.142%
18	10.510	1428	1432	1436	rBV	1408626	1390549	50.42%	5.625%
19	10.645	1451	1455	1463	rBV	86657	106161	3.85%	0.429%
20	11.092	1527	1531	1534	rBV2	62814	51759	1.88%	0.209%
21	11.204	1546	1550	1553	rBV	909915	754513	27.36%	3.052%
22	11.527	1600	1605	1610	rVB2	98579	90435	3.28%	0.366%
23	11.704	1632	1635	1638	rBV2	133211	110089	3.99%	0.445%
24	11.745	1638	1642	1645	rBV2	43871	48755	1.77%	0.197%
25	11.939	1673	1675	1677	rBV2	84609	72636	2.63%	0.294%
26	11.957	1677	1678	1681	rVB	68458	36114	1.31%	0.146%
27	12.233	1722	1725	1727	rBV	50522	39481	1.43%	0.160%
28	12.292	1733	1735	1737	rBV3	38945	39567	1.43%	0.160%
29	12.316	1737	1739	1741	rVB2	41471	32687	1.19%	0.132%
30	12.410	1751	1755	1758	rBV	54354	47249	1.71%	0.191%
31	12.510	1769	1772	1775	rVB	167795	133179	4.83%	0.539%
32	12.616	1786	1790	1796	rBV3	163410	301095	10.92%	1.218%
33	12.786	1815	1819	1823	rBV	1731817	1738311	63.03%	7.031%
34	13.327	1908	1911	1914	rBV	76799	66681	2.42%	0.270%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.692	1969	1973	1981	rVB	138819	158714	5.75%	0.642%
36	13.833	1992	1997	2000	rBV	713855	675412	24.49%	2.732%
37	14.321	2078	2080	2084	rBV	47937	55784	2.02%	0.226%
38	14.621	2128	2131	2138	rBV3	32629	51947	1.88%	0.210%
39	14.751	2150	2153	2158	rVB3	53184	60742	2.20%	0.246%
40	14.951	2181	2187	2191	rBV2	63887	103795	3.76%	0.420%
41	15.115	2212	2215	2218	rBV2	38248	48045	1.74%	0.194%
42	15.233	2230	2235	2239	rBV	549087	622861	22.58%	2.519%
43	15.686	2308	2312	2316	rBV2	41391	60440	2.19%	0.244%

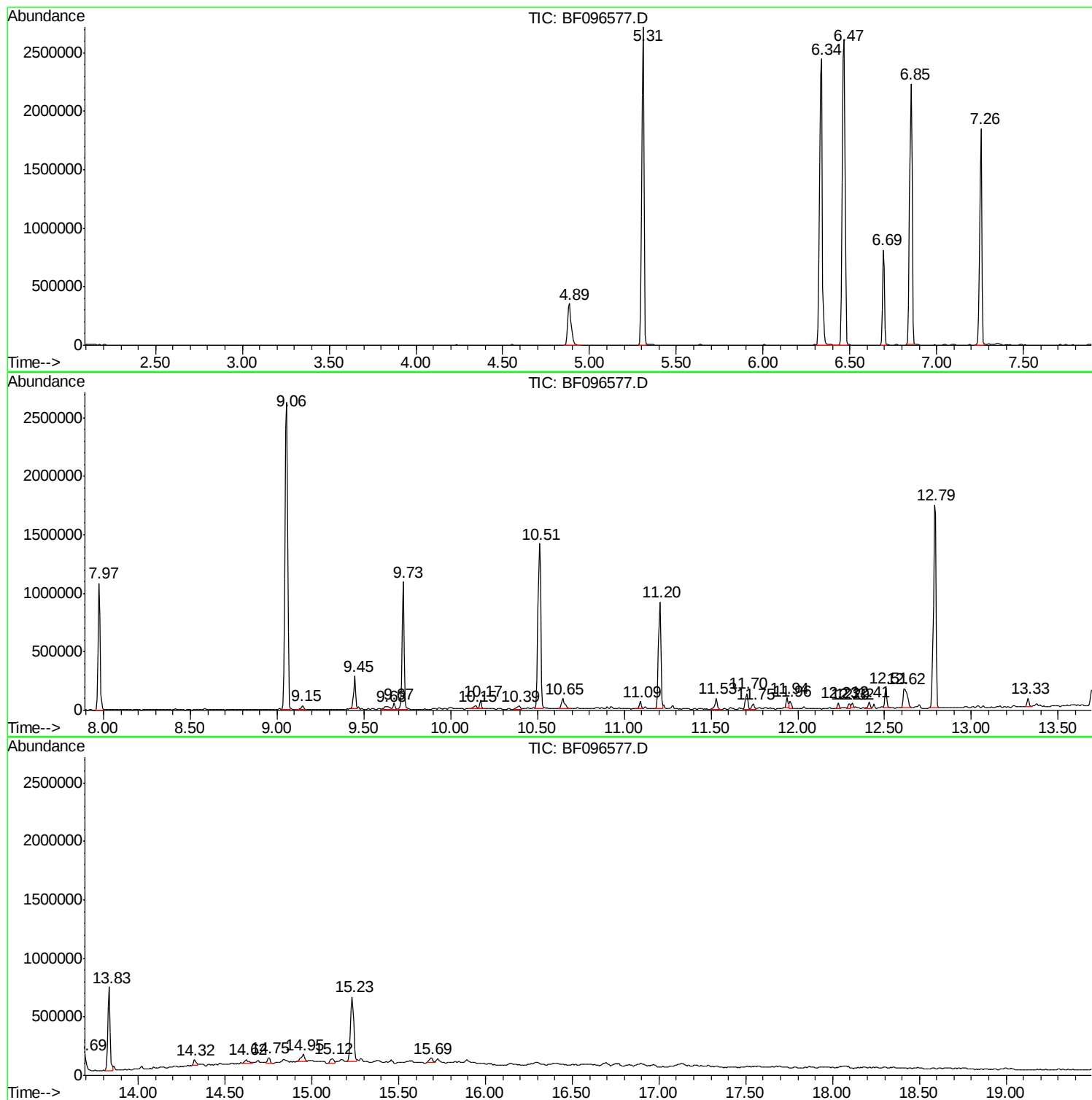
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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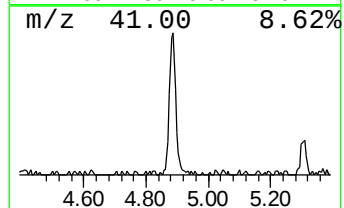
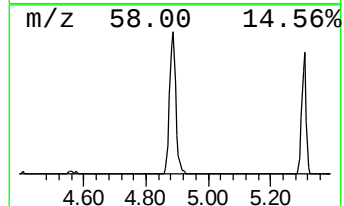
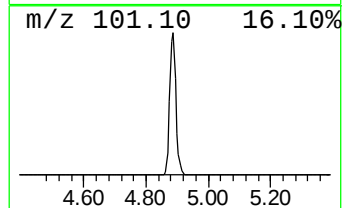
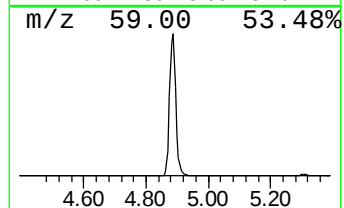
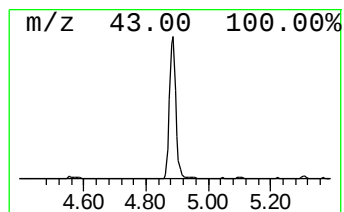
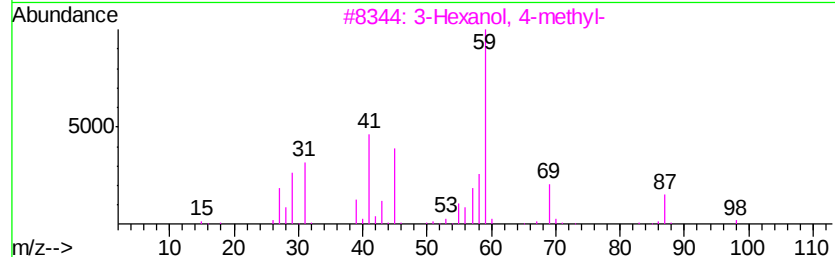
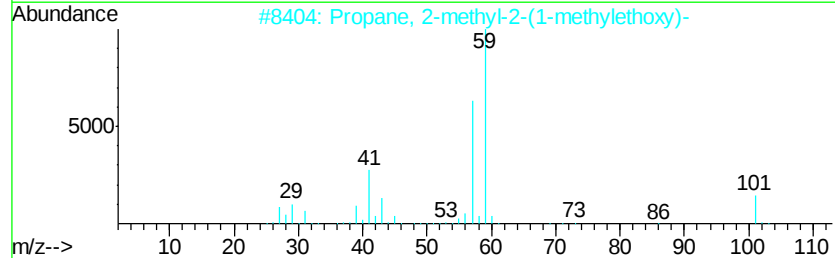
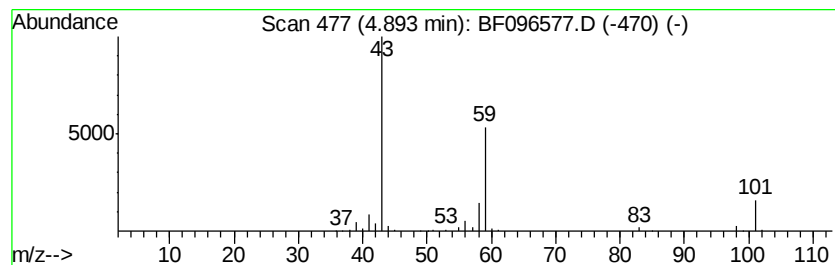
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	14.02 ng	481900	1,4-Dichlorobenzene-d4	6.69

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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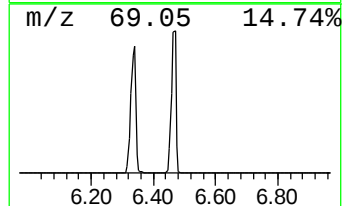
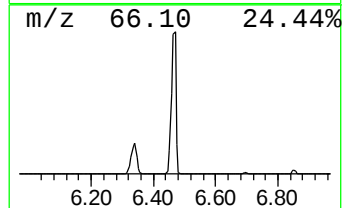
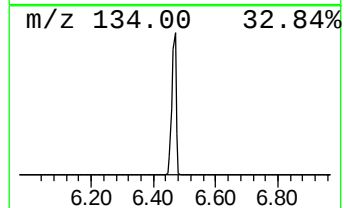
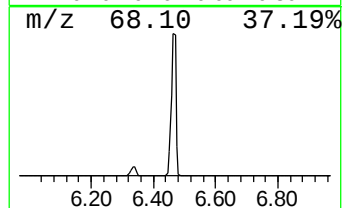
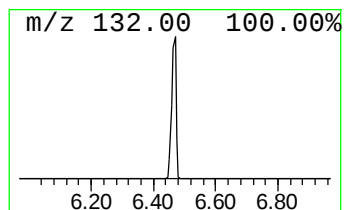
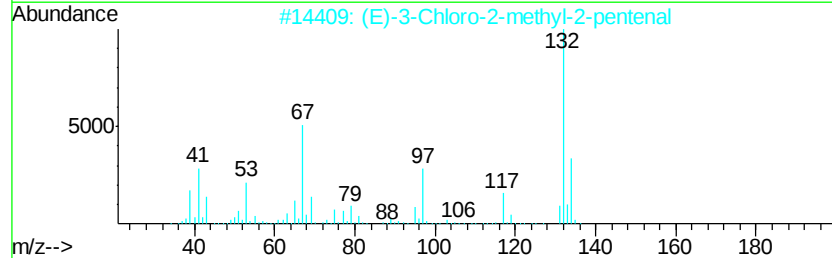
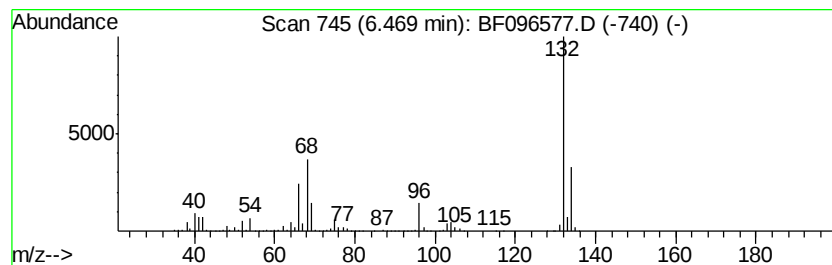
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	77.29 ng	2656280	1,4-Dichlorobenzene-d4	6.69

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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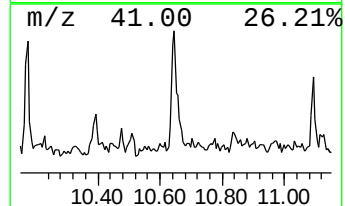
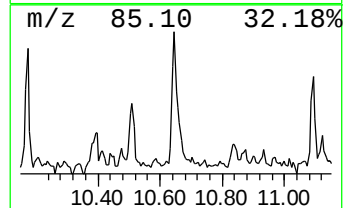
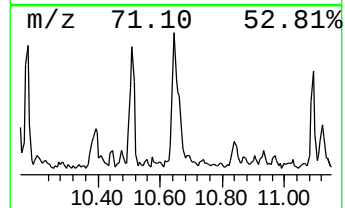
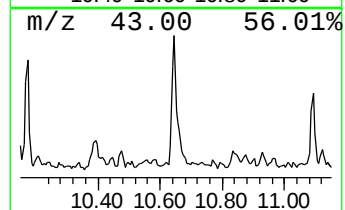
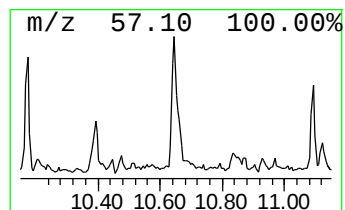
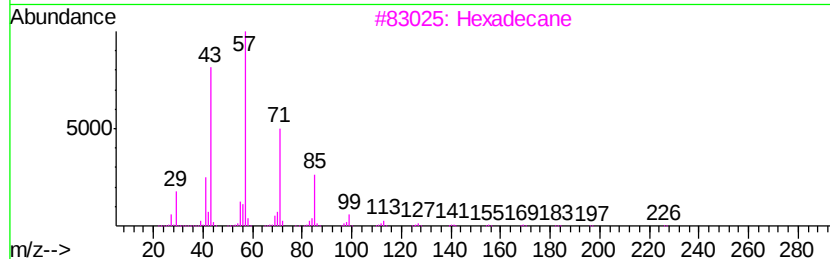
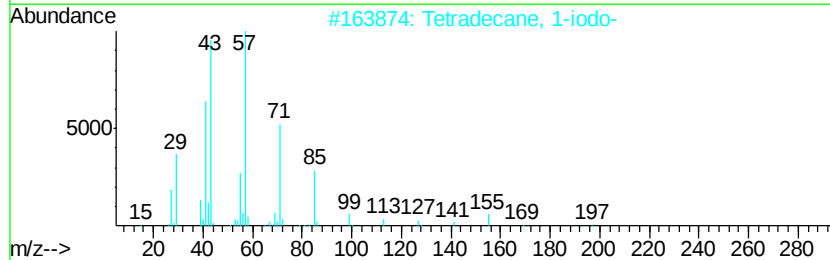
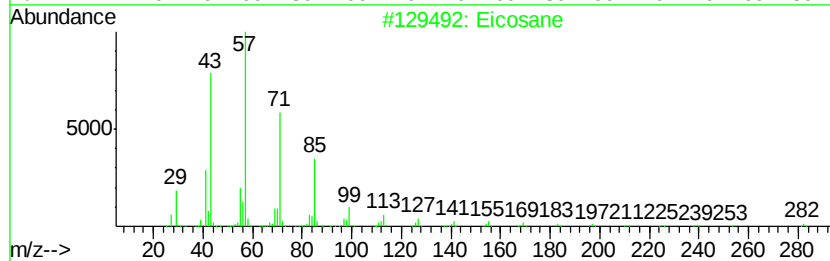
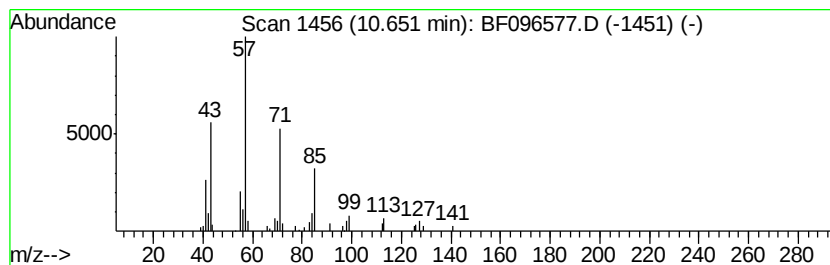
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	2.81 ng	106161	Phenanthrene-d10	11.20

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	90
3	Hexadecane		226	C16H34	000544-76-3	90
4	Tridecane		184	C13H28	000629-50-5	86
5	Pentadecane		212	C15H32	000629-62-9	86



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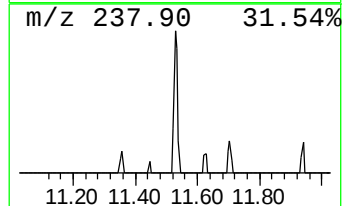
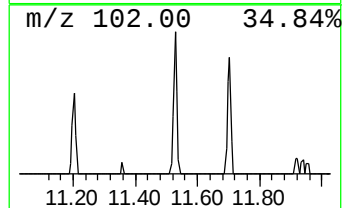
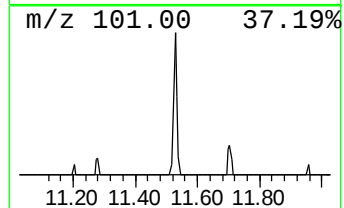
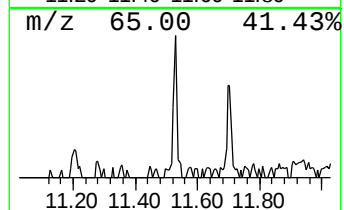
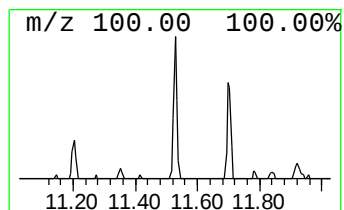
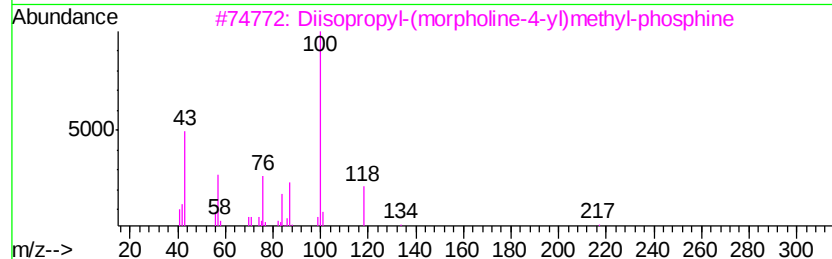
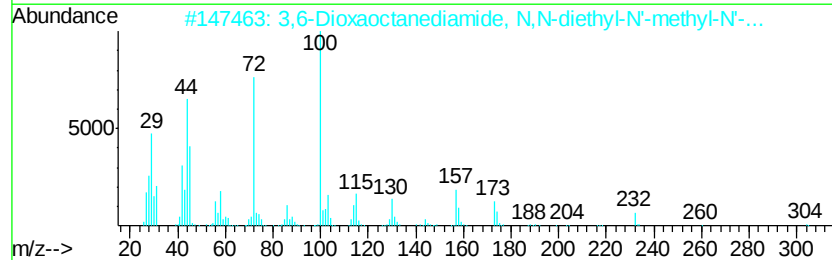
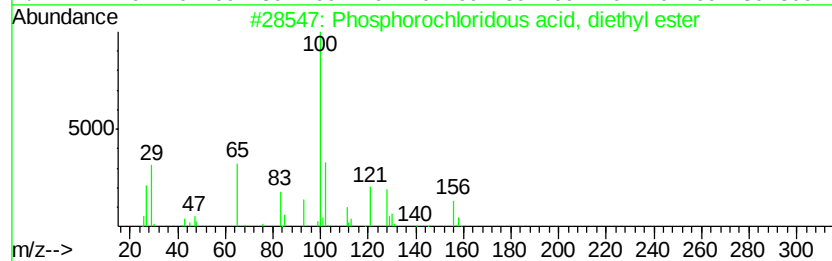
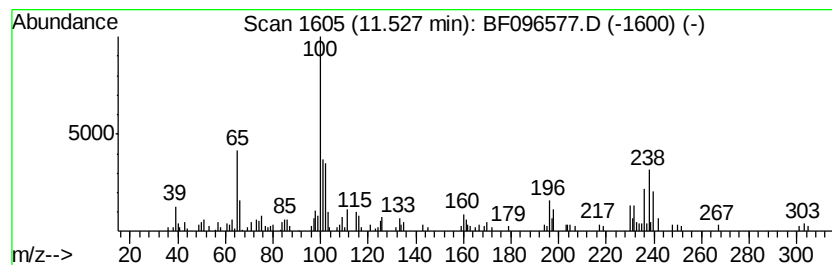
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown11.53 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.53	2.40 ng	90435	Phenanthrene-d10	11.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phosphorochloridous acid, diethy...	156	C4H10ClO2P	000589-57-1	36
2		3,6-Dioxaoctanediamide, N,N-diet...	304	C13H24N2O6	1000196-53-4	25
3		Diisopropyl-(morpholine-4-yl)met...	217	C11H24N0P	062474-29-7	10
4		Perfluoro[1,2-bis(tetrahydrofury...	458	C10H2F16O2	1000222-75-5	9
5		3-Morpholino-1,2-propanediol	161	C7H15NO3	006425-32-7	9



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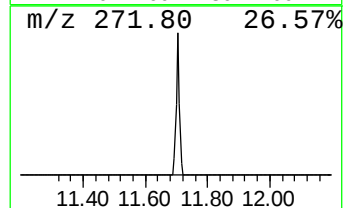
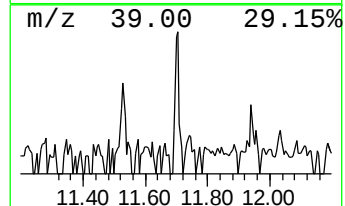
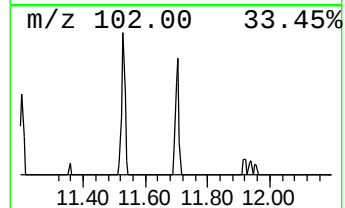
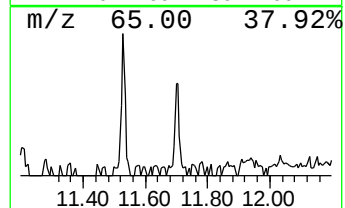
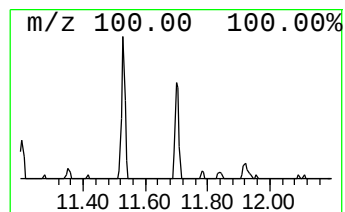
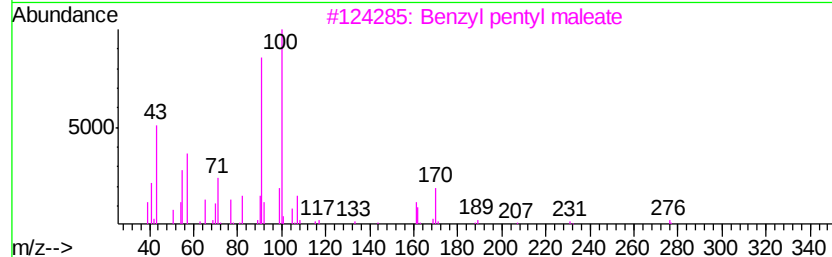
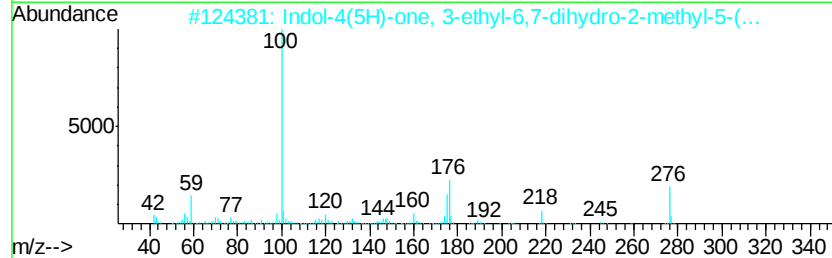
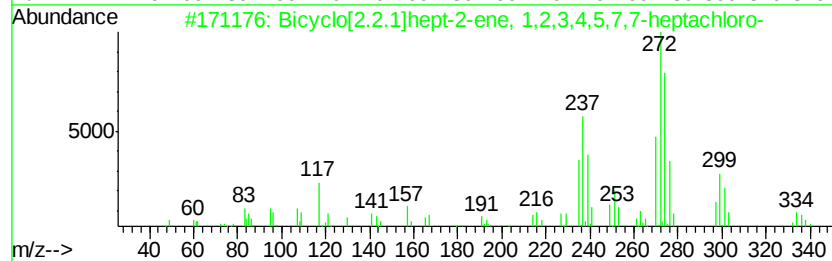
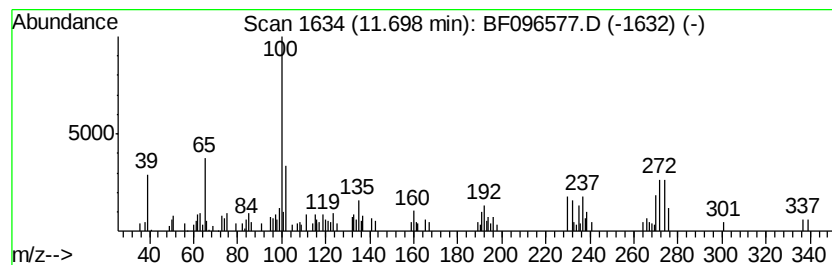
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Peak Number 6 Bicyclo[2.2.1]hept-2-ene, 1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.70	2.92 ng	110089	Phenanthrene-d10	11.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Bicyclo[2.2.1]hept-2-ene, 1,2,3,...	332 C7H3Cl7	005202-36-8	62
2	Indol-4(5H)-one, 3-ethyl-6,7-dih...	276 C16H24N2O2	007416-34-4	10
3	Benzyl pentyl maleate	276 C16H20O4	105113-86-8	9
4	Phosphorochloridous acid, diethy...	156 C4H10ClO2P	000589-57-1	9
5	(Tetrafluorosuccinimido)sulfur p...	297 C4F9N02S	080409-49-0	9



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096577.D
Acq On : 7 Jul 2017 23:40
Operator : SJ/MA
Sample : I4070-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-070517-D

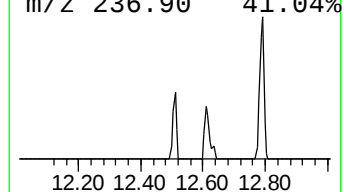
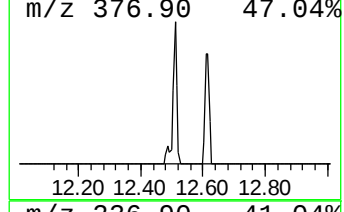
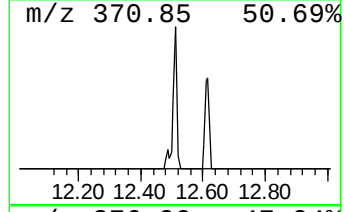
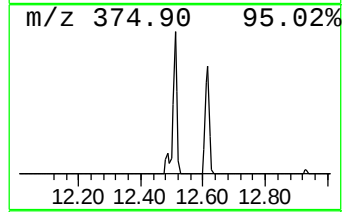
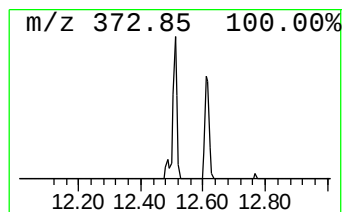
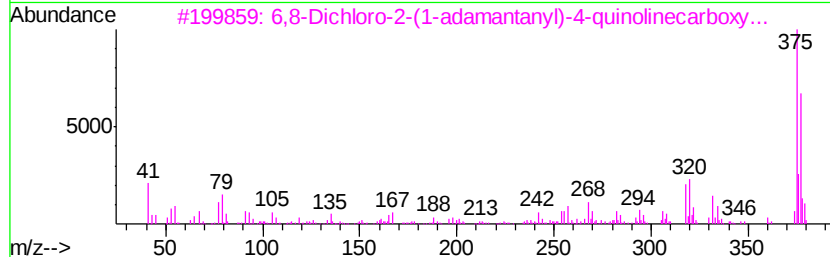
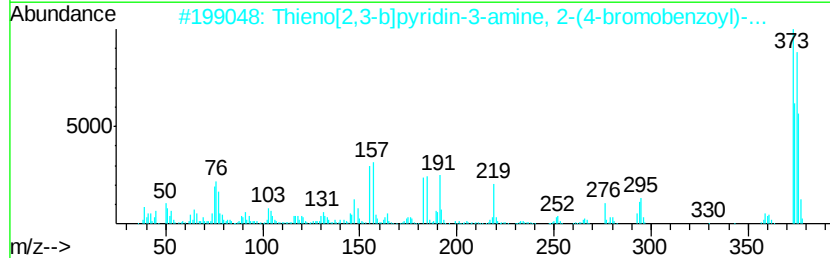
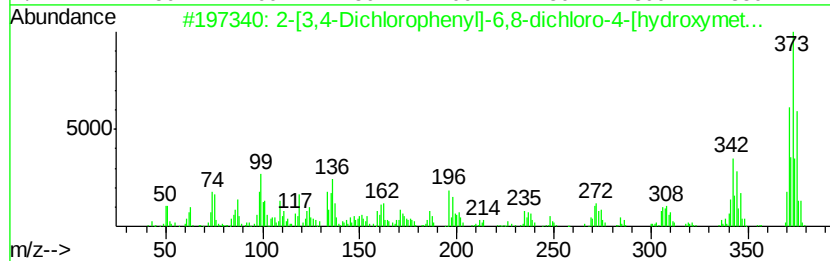
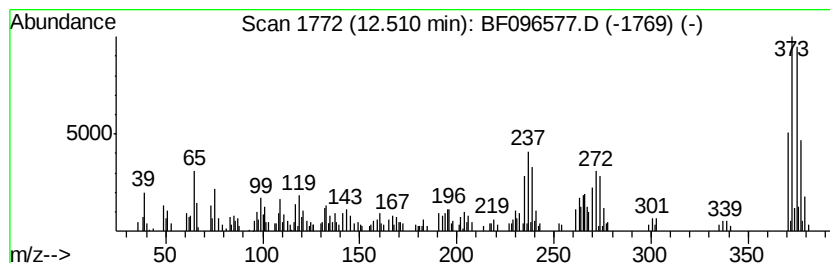
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.51 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	3.53 ng	133179	Phenanthrene-d10	11.20

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-[3,4-Dichlorophenyl]-6,8-dichl...	371	C16H9Cl4NO	038599-01-8	23	
2	Thieno[2,3-b]pyridin-3-amine, 2-...	374	C17H15BrN2OS	312316-45-3	17		
3	6,8-Dichloro-2-(1-adamantanyl)-4...	375	C20H19Cl2N02	049647-91-8	10		
4	2,5-Difluorobenzamide, N-(2-iodo...	373	C14H10F2INO	1000358-05-2	10		
5	Quinoline, N-oxy-4-[2-[3-[p-chlo...	373	C23H16ClN02	1000211-32-6	9		



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Acq On : 7 Jul 2017 23:40
Operator : SJ/MA
Sample : I4070-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-070517-D

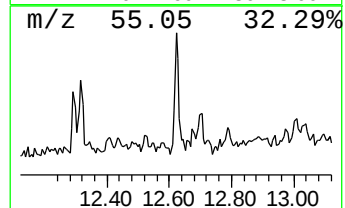
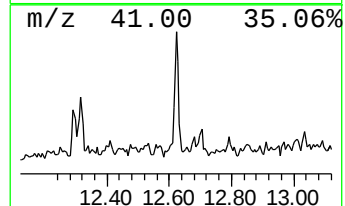
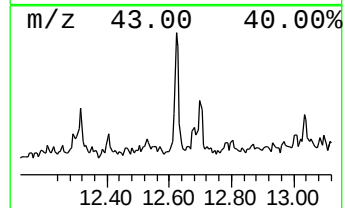
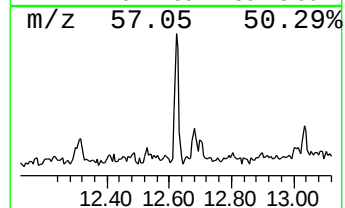
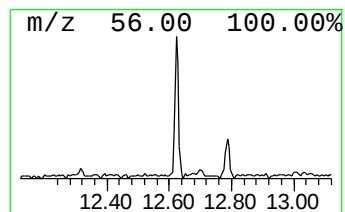
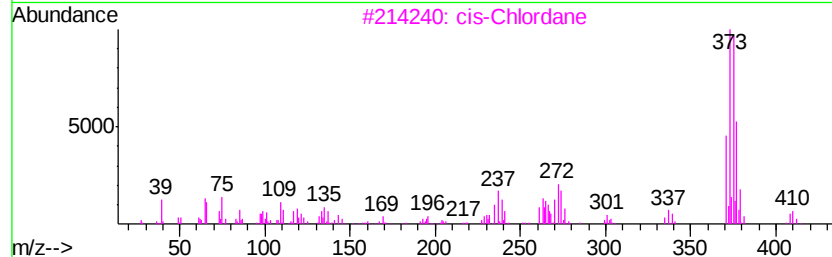
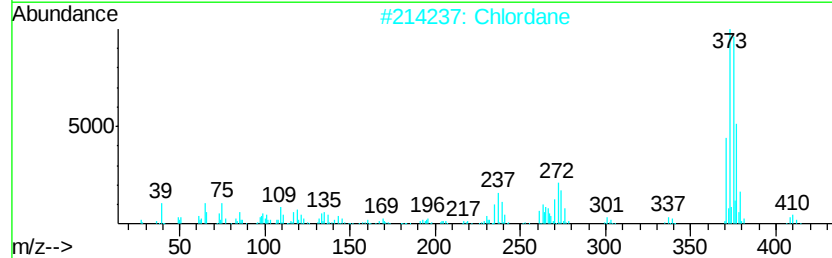
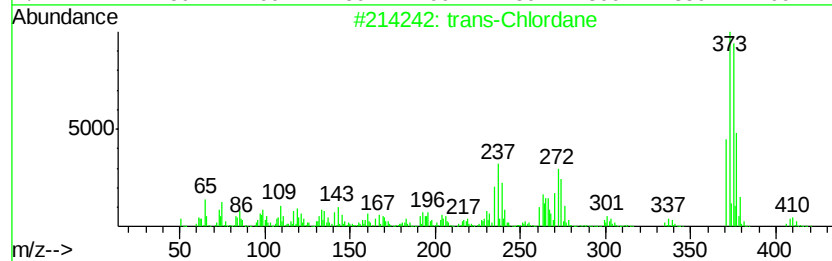
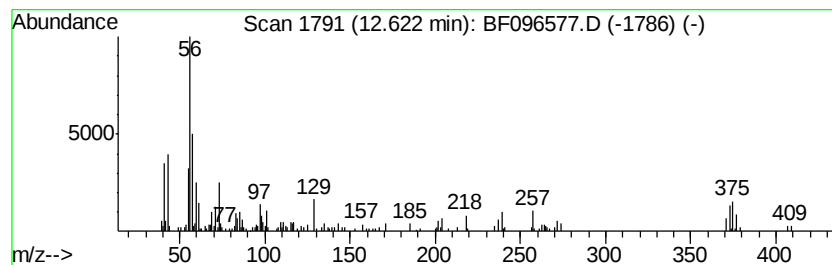
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 trans-Chlordane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.62	8.92 ng	301095	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	trans-Chlordane	406	C10H6Cl8	005103-74-2	99
2		Chlordane	406	C10H6Cl8	000057-74-9	99
3		cis-Chlordane	406	C10H6Cl8	005103-71-9	99
4		4,7-Methanoindene, 1,2,3,5,6,7,8...	406	C10H6Cl8	1000017-10-9	87
5		1-Piperidinecarbodithioic acid, ...	408	C12H10Cl3F3N2S2	1000305-31-5	12



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096577.D
Acq On : 7 Jul 2017 23:40
Operator : SJ/MA
Sample : I4070-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-070517-D

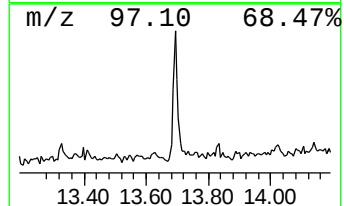
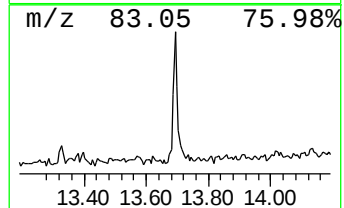
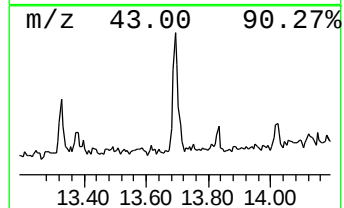
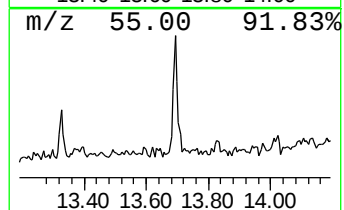
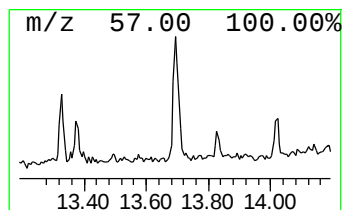
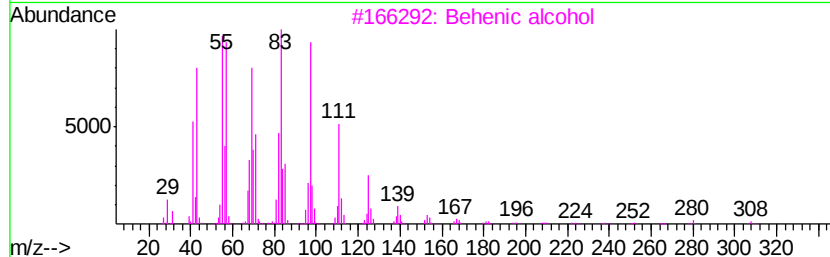
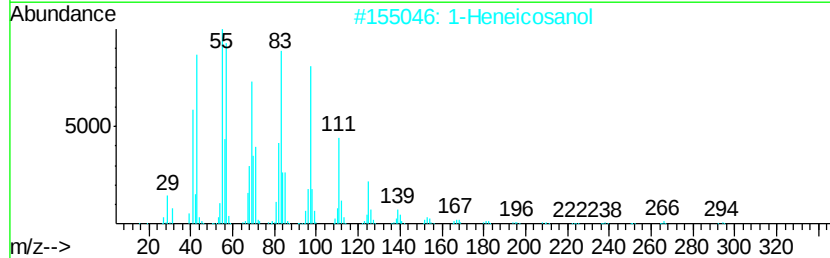
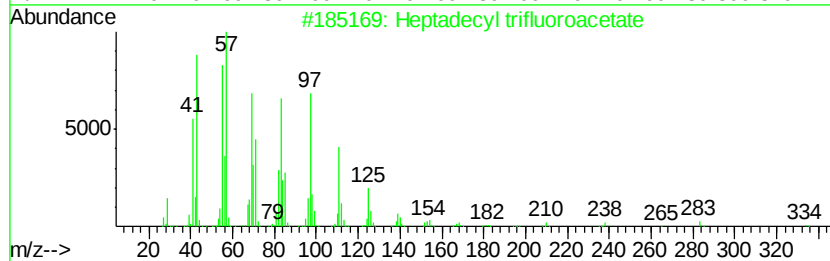
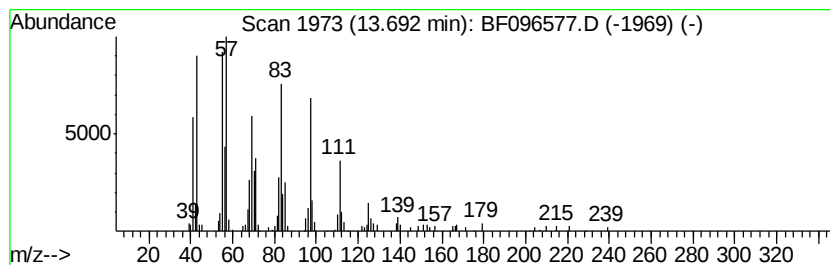
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	4.70 ng	158714	Chrysene-d12	13.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	93
3		Behenic alcohol	326	C22H46O	000661-19-8	93
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Docosene	308	C22H44	001599-67-3	91



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
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Operator : SJ/MA
Sample : I4070-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
AU-05-070517-D

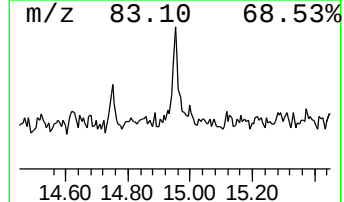
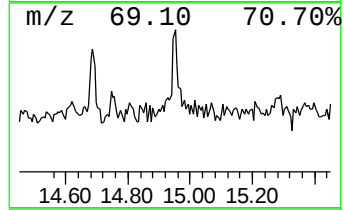
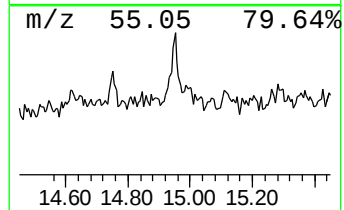
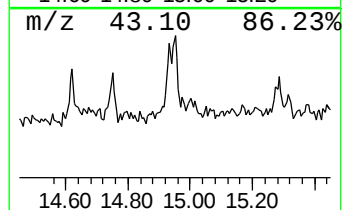
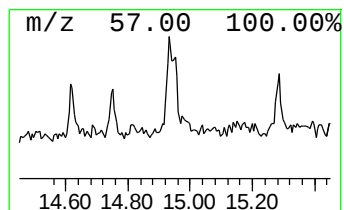
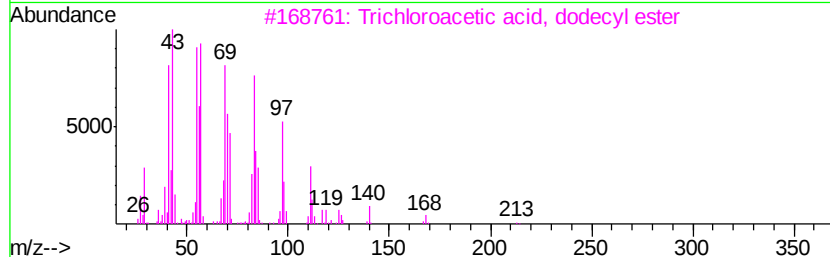
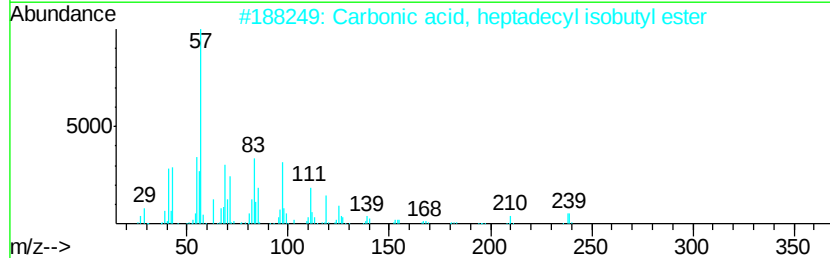
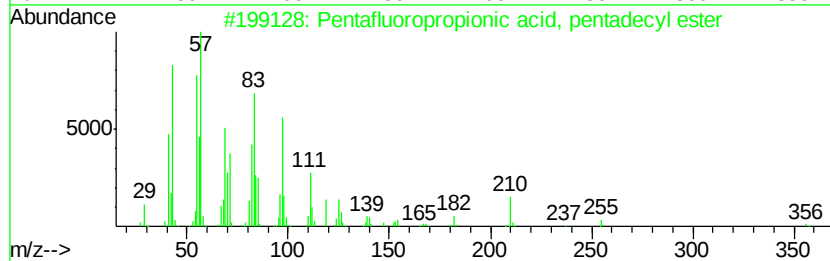
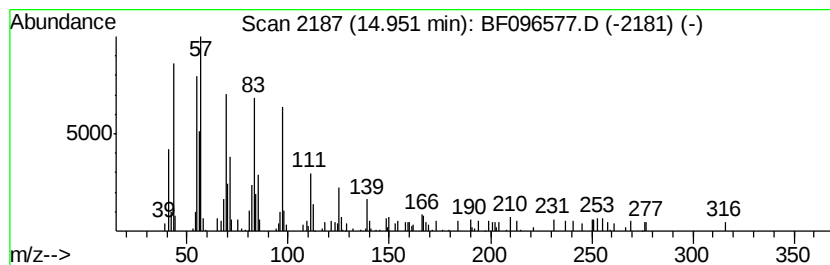
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.33 ng	103795	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
2		Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	86
3		Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	83
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5		2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	76



Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
Data File : BF096577.D
Acq On : 7 Jul 2017 23:40
Operator : SJ/MA
Sample : I4070-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.89	14.0	ng	481900	1	6.69	687362	20.0
unknown6.47	6.47	77.3	ng	2656280	1	6.69	687362	20.0
Eicosane	10.65	2.8	ng	106161	4	11.20	754513	20.0
unknown11.53	11.53	2.4	ng	90435	4	11.20	754513	20.0
Bicyclo[2.2.1]hep...	11.70	2.9	ng	110089	4	11.20	754513	20.0
unknown12.51	12.51	3.5	ng	133179	4	11.20	754513	20.0
trans-Chlordane	12.62	8.9	ng	301095	5	13.83	675412	20.0
Heptadecyl triflu...	13.69	4.7	ng	158714	5	13.83	675412	20.0
Pentafluoropropio...	14.95	3.3	ng	103795	6	15.23	622861	20.0