

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
 Data File : BF096178.D
 Acq On : 24 Jun 2017 1:19
 Operator : SJ/MA
 Sample : I3657-11
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-105D

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-BF060517.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	1.540	7	9	43	rVB	474968	917635	47.76%	6.853%
2	4.428	496	500	506	rBV4	14378	33148	1.73%	0.248%
3	4.810	560	565	576	rBV2	31189	58743	3.06%	0.439%
4	5.157	621	624	652	rBV	194249	617467	32.14%	4.611%
5	6.869	911	915	920	rBV	109037	233724	12.17%	1.745%
6	6.922	920	924	944	rVB	742509	1504006	78.28%	11.232%
7	7.257	977	981	991	rBV	252552	352829	18.37%	2.635%
8	7.492	1016	1021	1036	rBV	858744	1193165	62.11%	8.911%
9	8.186	1134	1139	1162	rBV	569624	959422	49.94%	7.165%
10	9.186	1301	1309	1312	rBV4	11447	21596	1.12%	0.161%
11	9.228	1312	1316	1323	rVV	17550	28641	1.49%	0.214%
12	9.292	1323	1327	1339	rVV	330406	461122	24.00%	3.444%
13	9.580	1368	1376	1388	rBV2	55818	101299	5.27%	0.757%
14	9.798	1409	1413	1423	rBV2	16934	42796	2.23%	0.320%
15	10.086	1454	1462	1468	rBV3	19215	35438	1.84%	0.265%
16	11.074	1624	1630	1645	rBV	1508568	1921196	100.00%	14.348%
17	11.469	1692	1697	1704	rBV2	18880	29598	1.54%	0.221%
18	11.774	1744	1749	1755	rBV	316648	404721	21.07%	3.022%
19	11.833	1755	1759	1763	rVV	61221	71116	3.70%	0.531%
20	11.886	1763	1768	1776	rVB7	11993	22677	1.18%	0.169%
21	12.057	1789	1797	1802	rBV3	15358	25988	1.35%	0.194%
22	12.116	1802	1807	1814	rBV2	368311	463808	24.14%	3.464%
23	12.216	1821	1824	1832	rVB2	20988	25314	1.32%	0.189%
24	12.839	1926	1930	1936	rBV	51300	63324	3.30%	0.473%
25	13.415	2023	2028	2042	rBV	573240	825037	42.94%	6.161%
26	14.462	2202	2206	2210	rBV2	15558	26566	1.38%	0.198%
27	14.510	2210	2214	2223	rVB	283008	388048	20.20%	2.898%
28	15.539	2386	2389	2396	rBV3	17461	26988	1.40%	0.202%
29	16.898	2615	2620	2624	rBV	1231632	1382695	71.97%	10.326%
30	18.156	2829	2834	2839	rBV3	18183	30787	1.60%	0.230%
31	18.245	2845	2849	2859	rVB	280637	376002	19.57%	2.808%
32	18.580	2902	2906	2919	rBV	177237	265280	13.81%	1.981%
33	19.103	2990	2995	2999	rBV	62708	68782	3.58%	0.514%
34	19.921	3130	3134	3143	rBV	230183	328559	17.10%	2.454%

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Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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35	20.268	3189	3193	3197	rBV	34952	40420	2.10%	0.302%
36	20.856	3289	3293	3297	rVB3	30796	42436	2.21%	0.317%

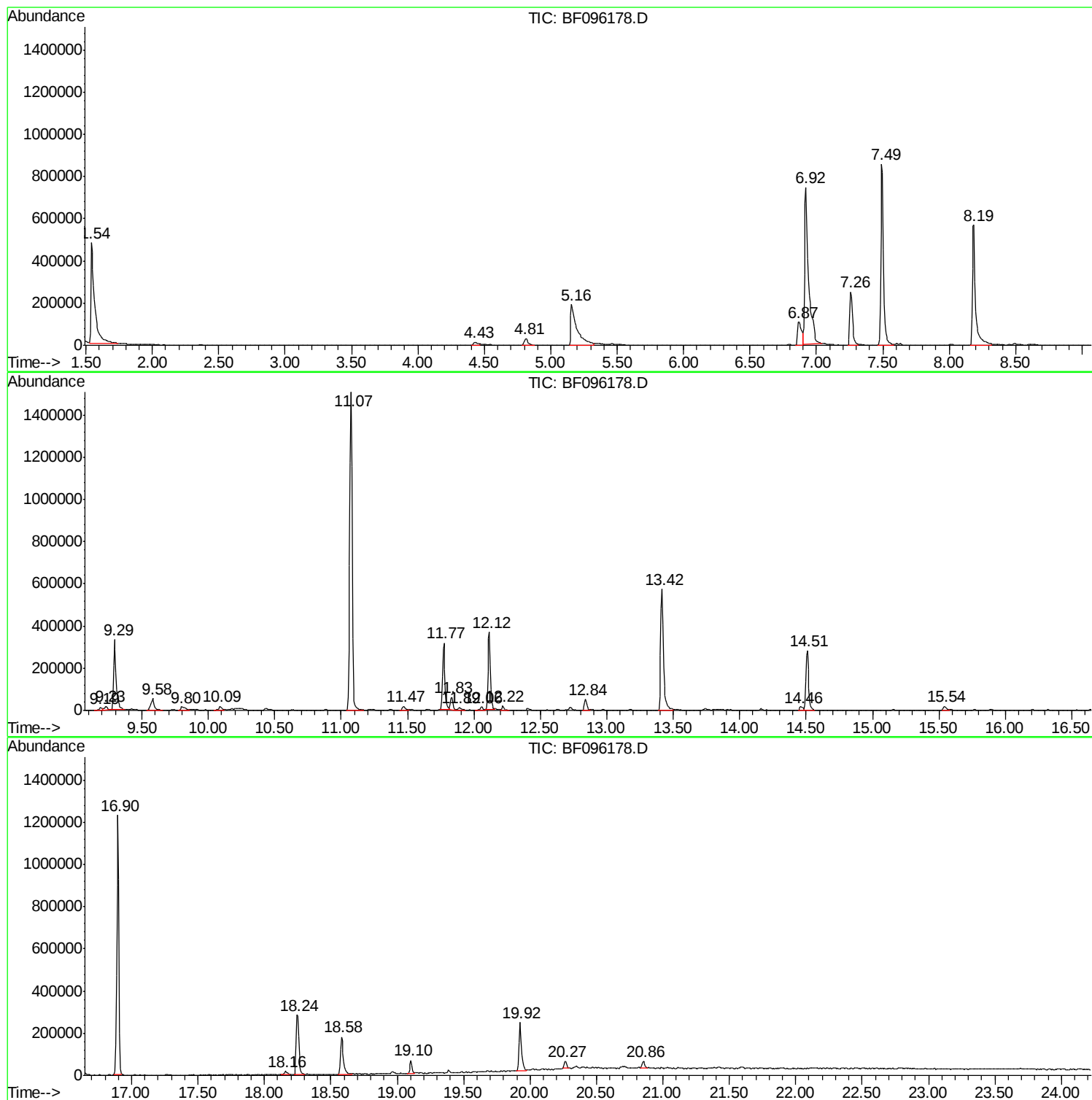
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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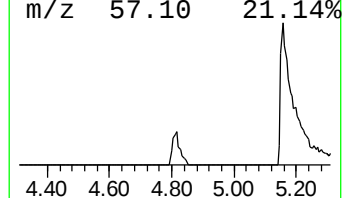
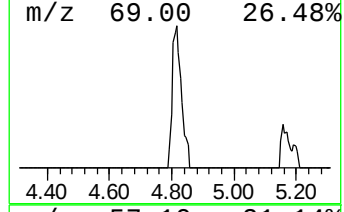
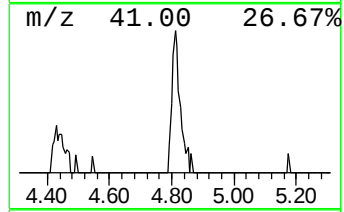
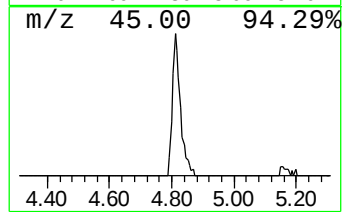
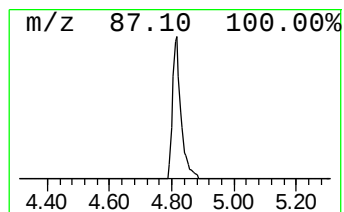
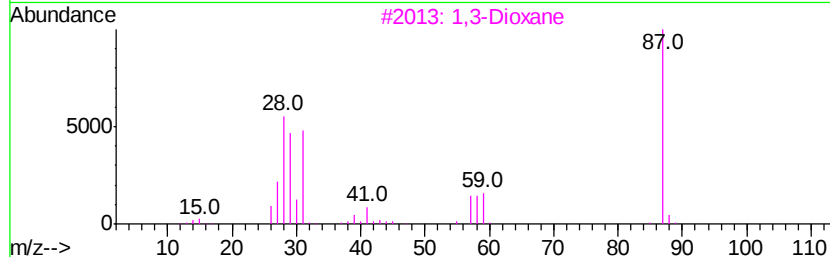
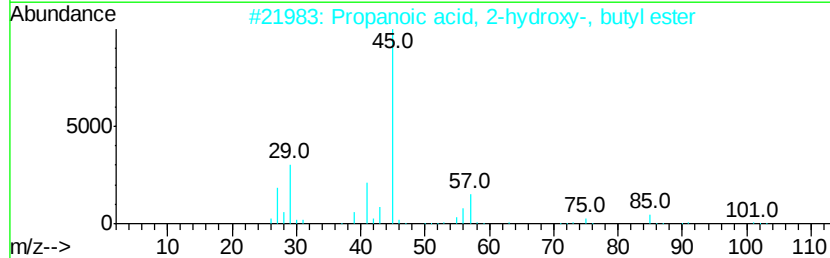
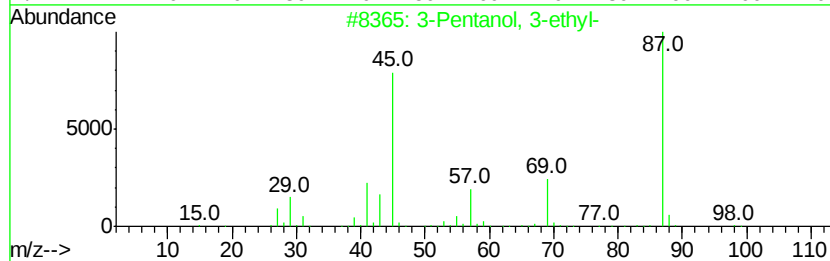
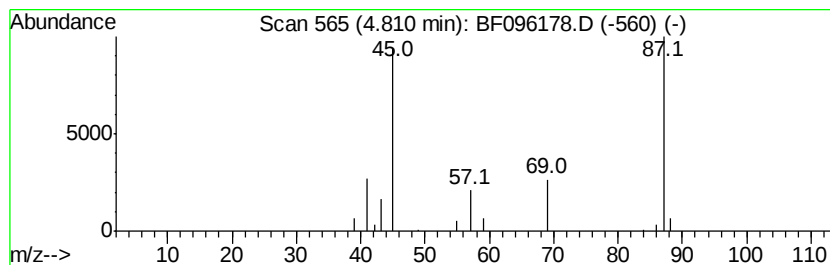
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Pentanol, 3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	3.33 ng	58743	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pentanol, 3-ethyl-	116	C7H16O	000597-49-9	74
2		Propanoic acid, 2-hydroxy-, butyl...	146	C7H14O3	000138-22-7	17
3		1,3-Dioxane	88	C4H8O2	000505-22-6	9
4		3-Pentanol, 2,2,4,4-tetramethyl-	144	C9H20O	014609-79-1	9
5		Hydroperoxide, 1,4-dioxan-2-yl	120	C4H8O4	004722-59-2	9



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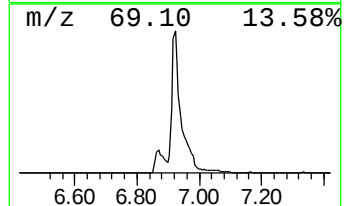
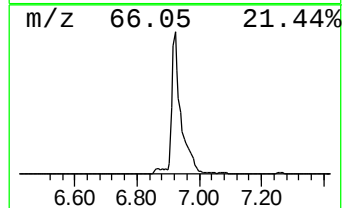
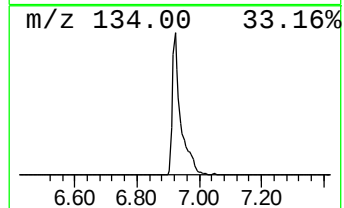
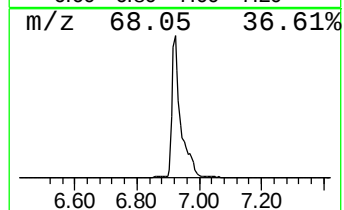
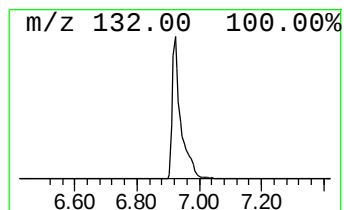
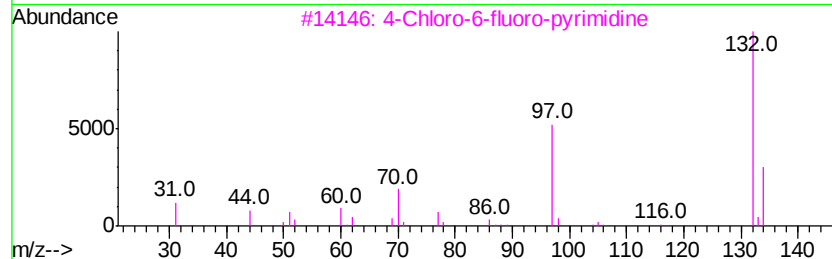
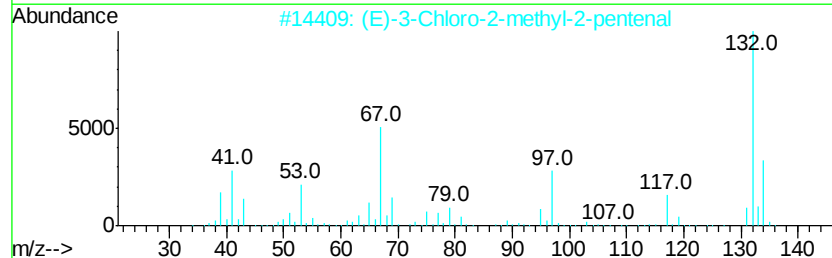
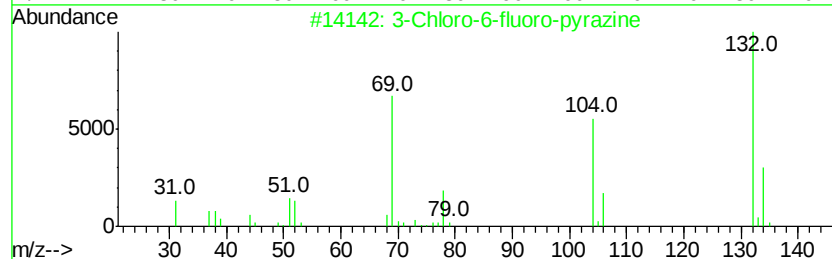
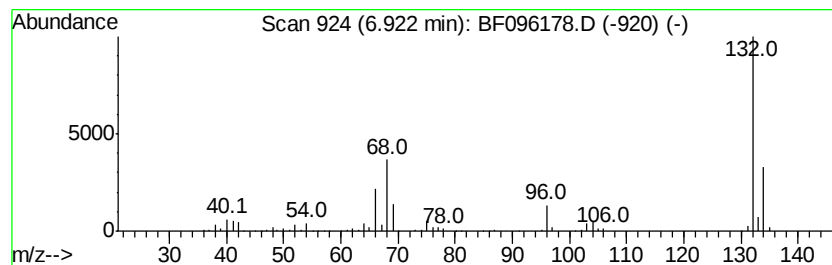
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	85.25 ng	1504010	1,4-Dichlorobenzene-d4	7.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	4		Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	2H-Cyclopenta[d]		pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]		pyrazine	132	C8H8N2	064608-60-2	9



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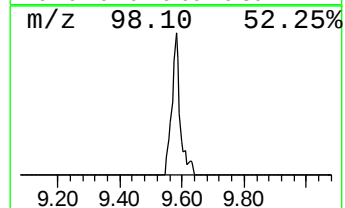
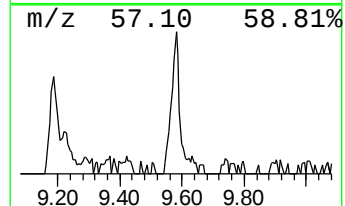
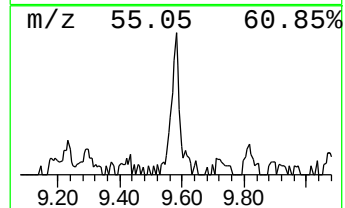
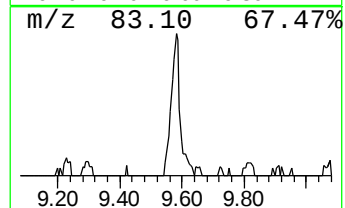
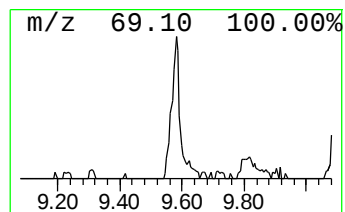
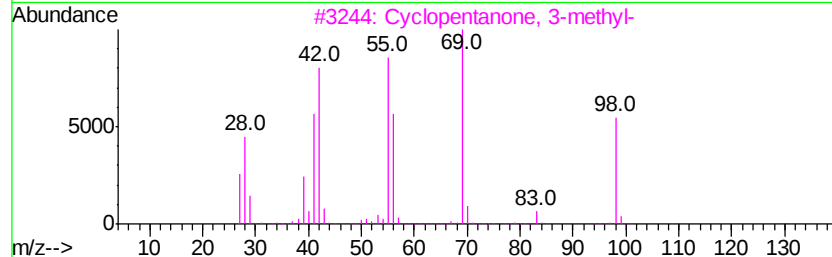
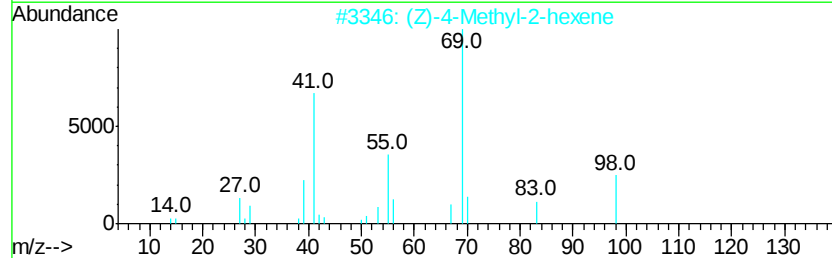
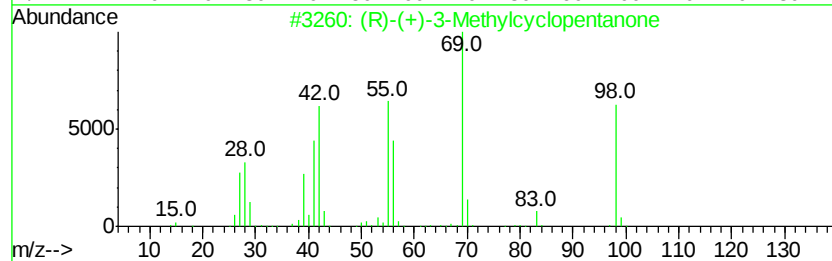
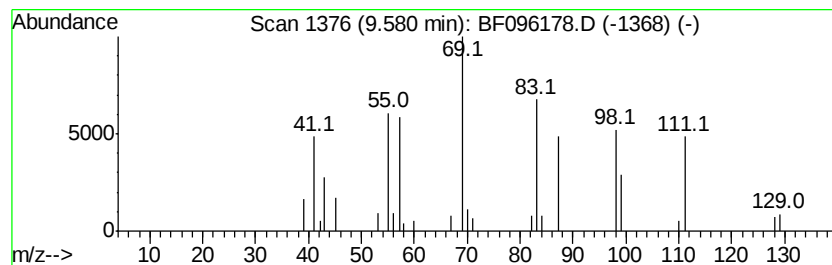
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown9.58 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.58	4.39 ng	101299	Naphthalene-d8	9.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(+)-3-Methylcyclopentanone			98	C6H10O	006672-30-6	35
2	(Z)-4-Methyl-2-hexene			98	C7H14	003683-19-0	35
3	Cyclopentanone, 3-methyl-			98	C6H10O	001757-42-2	35
4	Cyclohexane, 1-ethyl-2,4-dimethyl-			140	C10H20	061142-69-6	35
5	Cyclooctane, (1-methylpropyl)-			168	C12H24	016538-89-9	35



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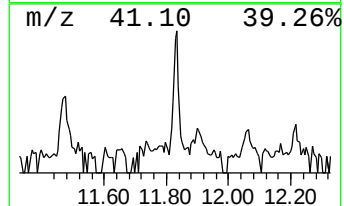
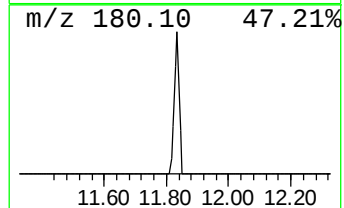
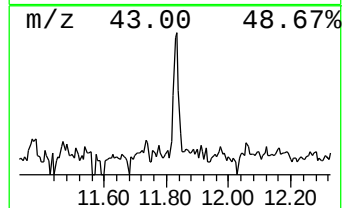
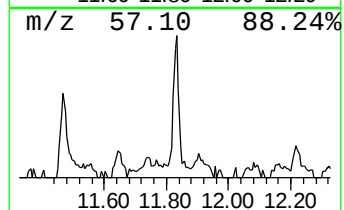
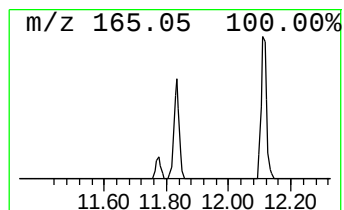
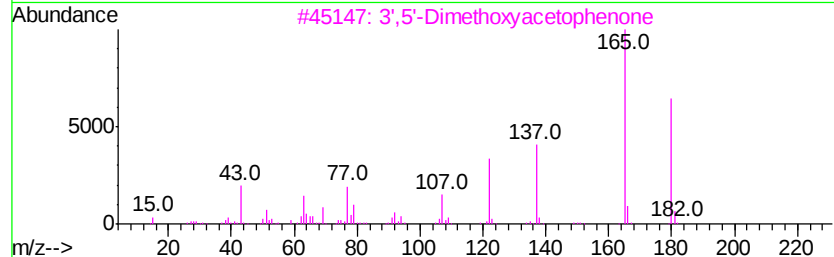
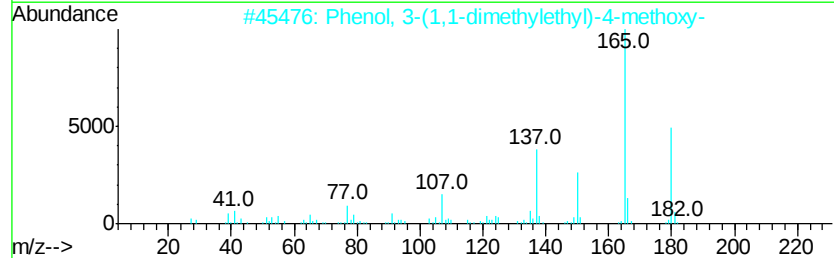
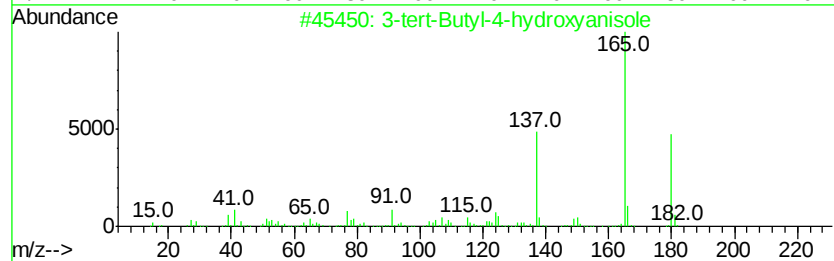
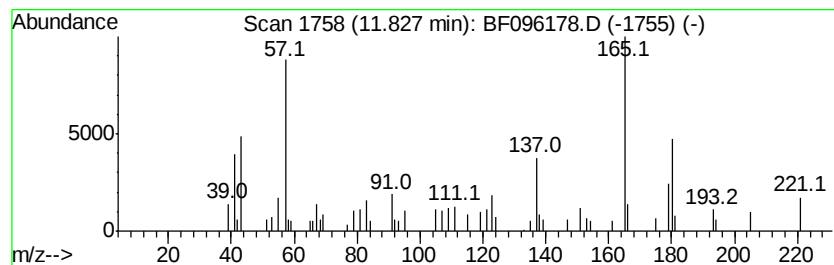
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 3-tert-Butyl-4-hydroxyanisole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	3.07 ng	71116	Acenaphthene-d10	12.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	70
2		Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	58
3		3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	52
4		Benzenethiol, 4-(1,1-dimethylethyl)-...	180	C11H16S	015570-10-2	49
5		Pentacyclo[6.4.0.1(1,8).1(2,7)]t...	180	C14H12	086120-84-5	46



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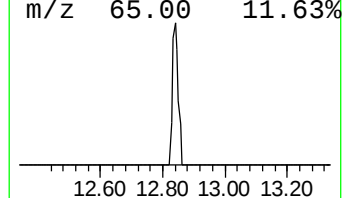
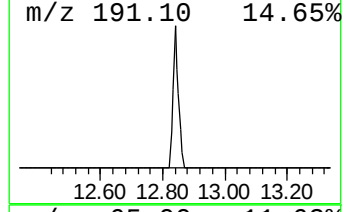
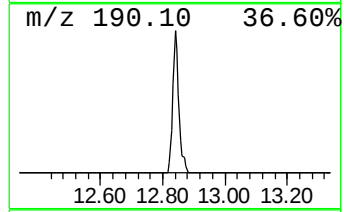
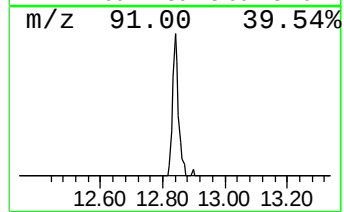
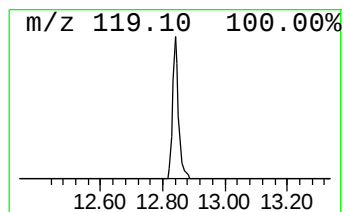
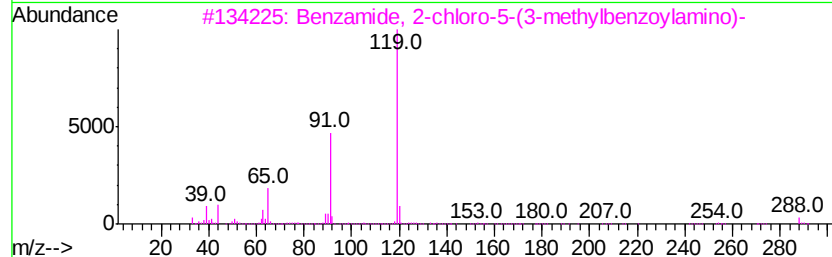
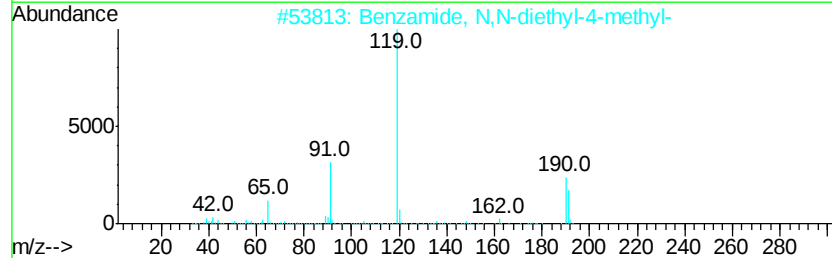
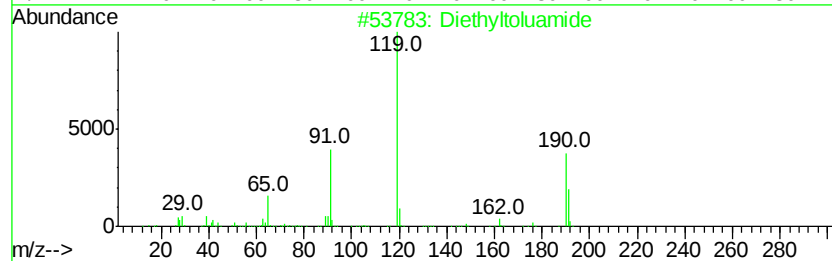
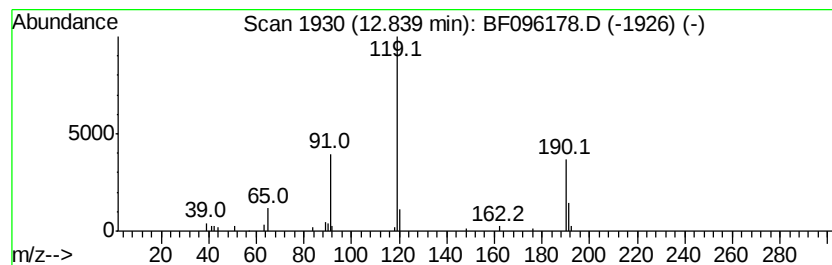
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Peak Number 7 Diethyltoluamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.73 ng	63324	Acenaphthene-d10	12.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2		Benzamide, N,N-diethyl-4-methyl-	191	C12H17NO	002728-05-4	91
3		Benzamide, 2-chloro-5-(3-methylb...	288	C15H13ClN2O2	349489-17-4	59
4		2-Methylbenzoic acid, 2-fluoroph...	230	C14H11FO2	1000325-60-5	59
5		2-Methylbenzoic acid, 3-chloroph...	246	C14H11ClO2	1000325-60-8	59



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096178.D
Acq On : 24 Jun 2017 1:19
Operator : SJ/MA
Sample : I3657-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

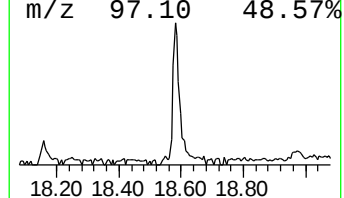
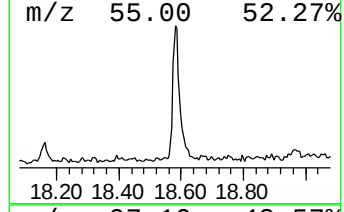
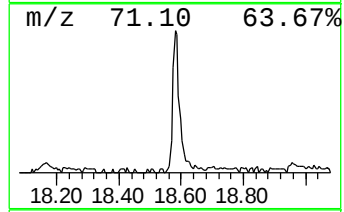
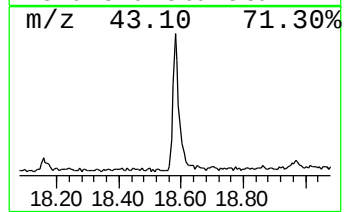
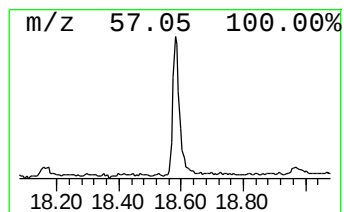
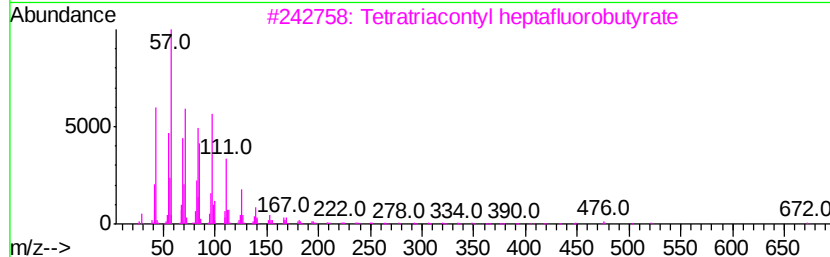
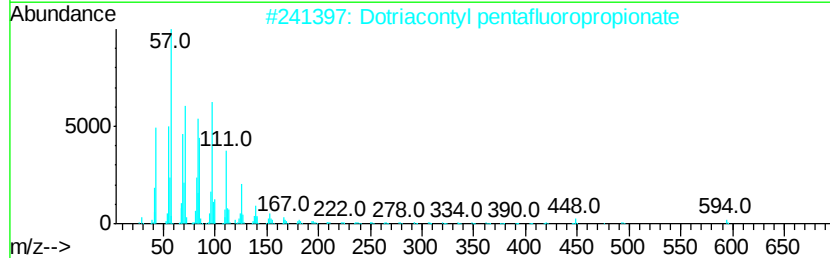
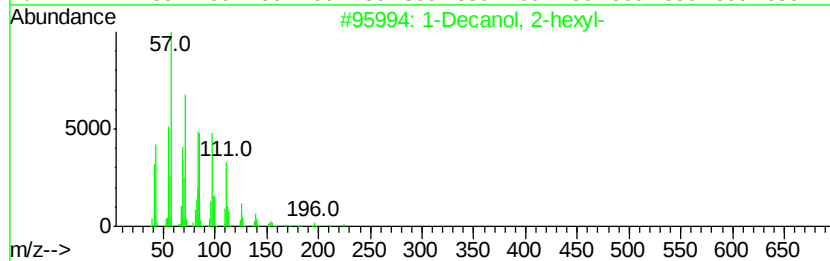
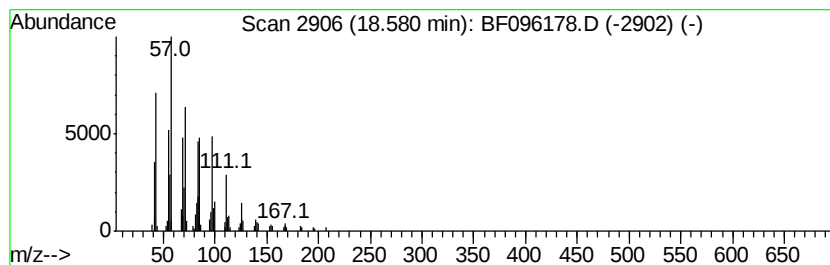
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Decanol, 2-hexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	14.11 ng	265280	Chrysene-d12	18.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
2		Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	91
3		Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	90
4		Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	90
5		Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	90



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Acq On : 24 Jun 2017 1:19
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Sample : I3657-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

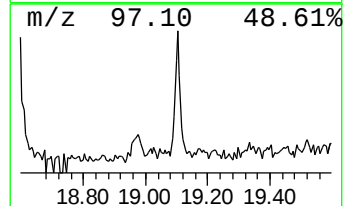
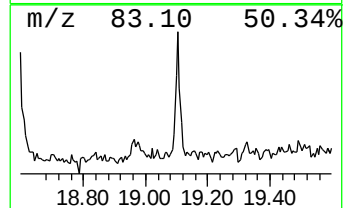
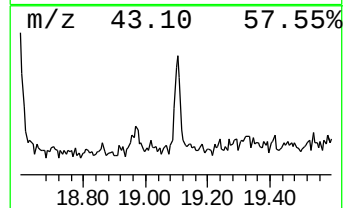
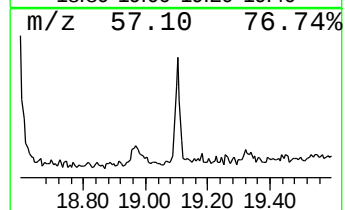
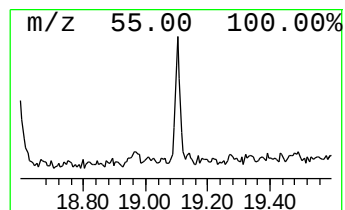
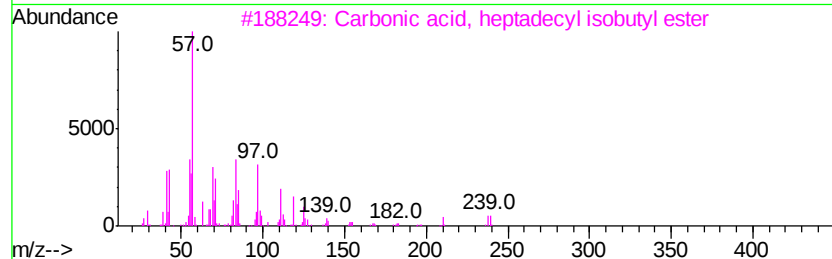
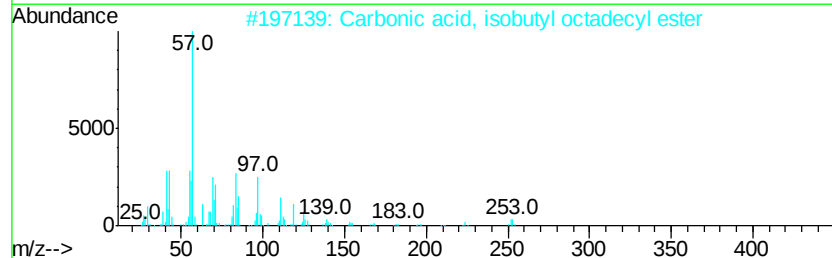
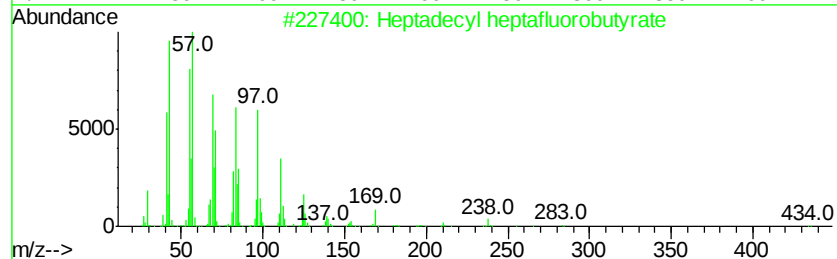
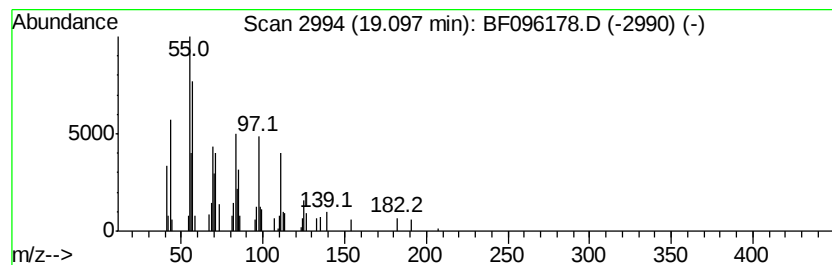
Instrument :
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ClientSampleId :
MW-105D

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.10	4.19 ng	68782	Perylene-d12	19.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
2	Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	87
3	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	87
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	74
5	Dotriacontyl trifluoroacetate	562	C34H65F3O2	1000351-75-4	70



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Operator : SJ/MA
Sample : I3657-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-105D

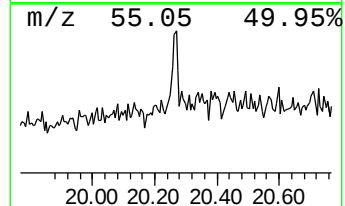
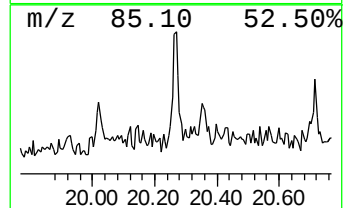
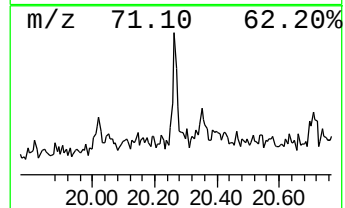
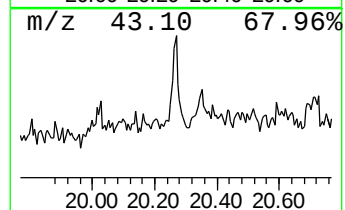
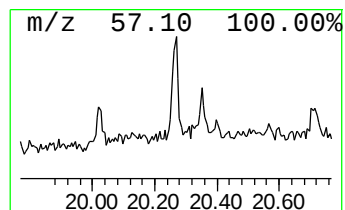
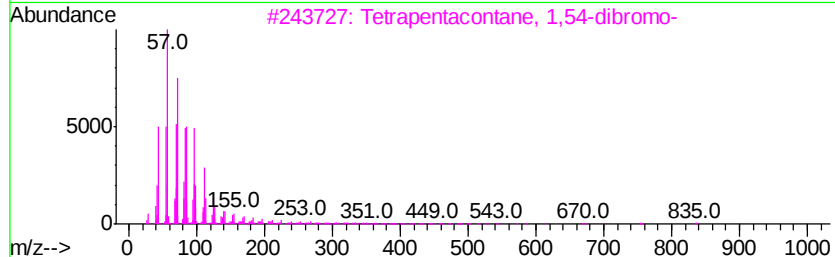
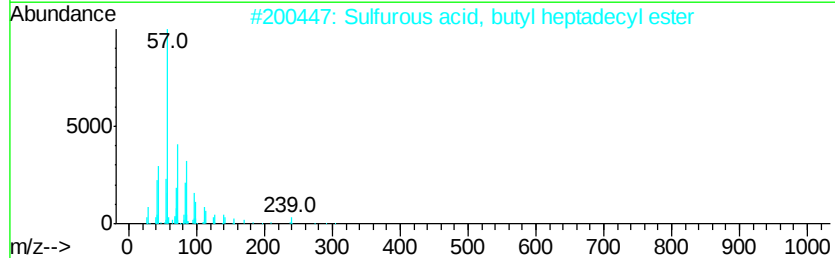
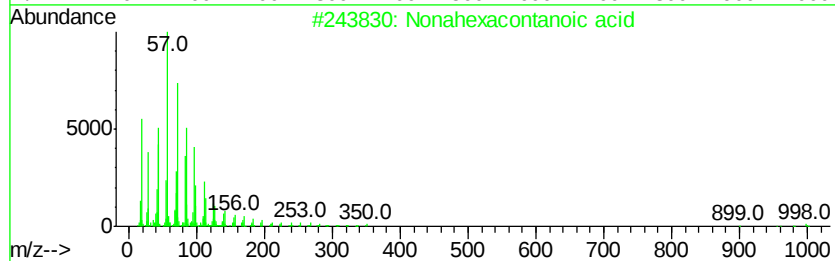
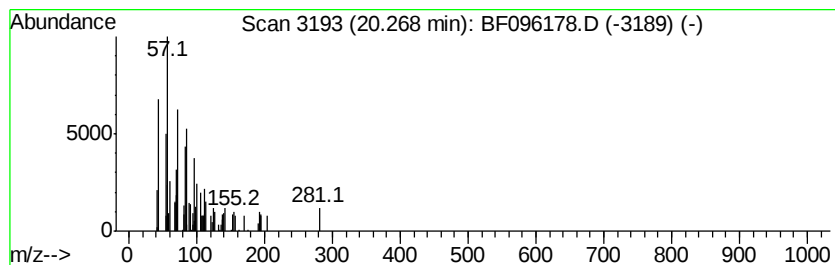
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Nonaheptacontanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.27	2.46 ng	40420	Perylene-d12	19.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonaheptacontanoic acid	999	C69H138O2	040710-32-5	76
2		Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	64
3		Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	58
4		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	49
5		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	49



Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
Data File : BF096178.D
Acq On : 24 Jun 2017 1:19
Operator : SJ/MA
Sample : I3657-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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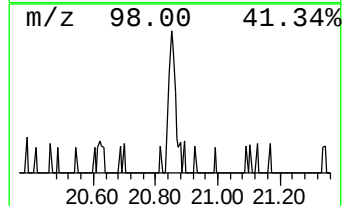
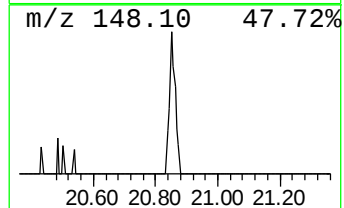
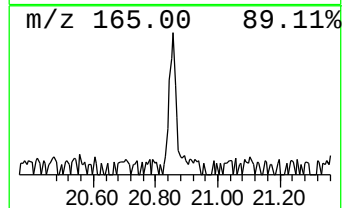
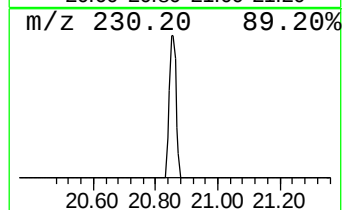
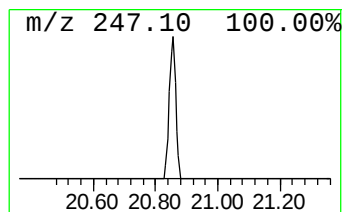
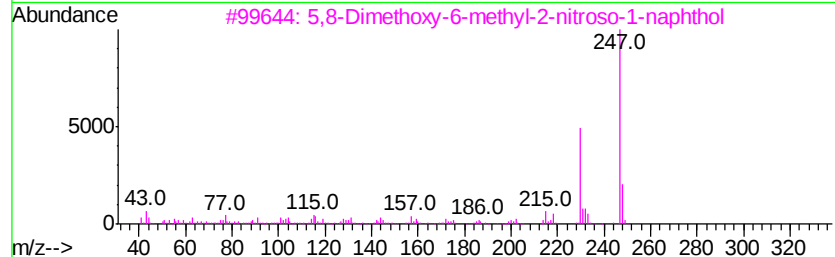
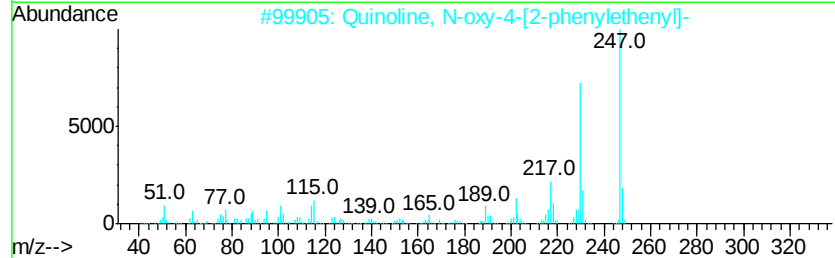
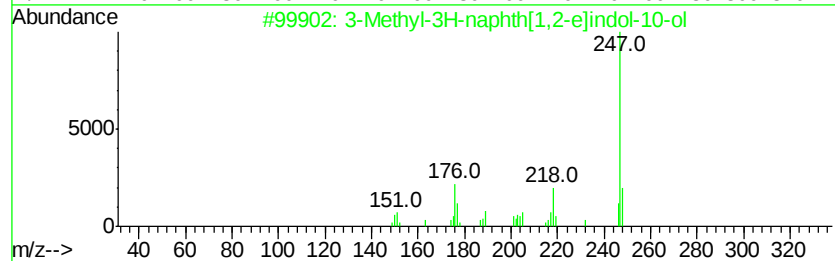
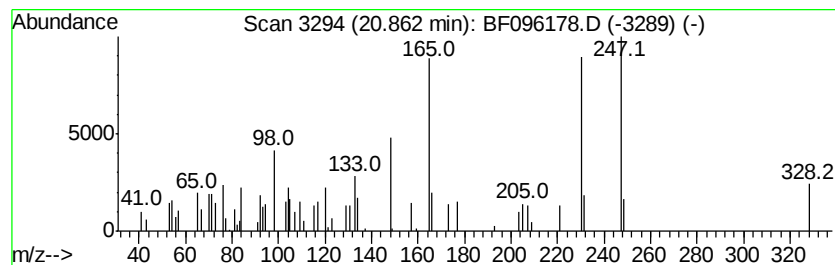
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown20.86 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	2.58 ng	42436	Perylene-d12	19.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Methyl-3H-naphth[1,2-e]indol-1...	247	C17H13NO	098033-21-7	27
2		Quinoline, N-oxv-4-[2-phenylethe...	247	C17H13NO	013244-22-9	25
3		5,8-Dimethoxy-6-methyl-2-nitroso...	247	C13H13NO4	099316-37-7	22
4		Isiondole-5-carboxamide, 2,3-dih...	328	C19H24N2O3	1000273-67-3	22
5		Thiazolo[2,3-c][1,2,4]triazole, ...	247	C12H13N3OS	1000303-64-4	16



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 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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
3-Pentanol, 3-ethyl-	4.81	3.3	ng	58743	1	7.26	352829	20.0
unknown6.92	6.92	85.3	ng	1504010	1	7.26	352829	20.0
unknown9.58	9.58	4.4	ng	101299	2	9.29	461122	20.0
3-tert-Butyl-4-hy...	11.83	3.1	ng	71116	3	12.12	463808	20.0
Diethyltoluamide	12.84	2.7	ng	63324	3	12.12	463808	20.0
1-Decanol, 2-hexyl-	18.58	14.1	ng	265280	5	18.25	376002	20.0
Heptadecyl hepta...	19.10	4.2	ng	68782	6	19.92	328559	20.0
Nonahexacontanoic...	20.27	2.5	ng	40420	6	19.92	328559	20.0
unknown20.86	20.86	2.6	ng	42436	6	19.92	328559	20.0