

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
 Data File : BF096819.D
 Acq On : 17 Jul 2017 15:09
 Operator : SJ/JU
 Sample : I4188-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B1(0-10)COMP

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-BF071317.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	4.781	472	475	484	rBV	170581	217540	10.73%	1.209%
2	5.216	545	549	563	rBV	1926512	2027950	100.00%	11.270%
3	6.263	722	727	737	rBV	1781628	1965021	96.90%	10.921%
4	6.381	743	747	750	rBV	2162924	1905281	93.95%	10.589%
5	6.610	782	786	789	rBV	761452	606083	29.89%	3.368%
6	6.769	808	813	816	rBV	1680173	1597001	78.75%	8.875%
7	6.951	839	844	848	rVB4	12442	24648	1.22%	0.137%
8	7.175	877	882	885	rBV	1427790	1365391	67.33%	7.588%
9	7.892	1000	1004	1007	rBV	1059209	876574	43.22%	4.872%
10	8.969	1182	1187	1190	rBV	2135073	2025727	99.89%	11.258%
11	9.357	1250	1253	1256	rBV	327915	262056	12.92%	1.456%
12	9.634	1296	1300	1304	rBV	924895	815406	40.21%	4.532%
13	10.086	1374	1377	1384	rVB2	39304	42948	2.12%	0.239%
14	10.416	1429	1433	1437	rBV	884912	806470	39.77%	4.482%
15	10.557	1453	1457	1464	rBV	37738	47967	2.37%	0.267%
16	11.004	1525	1533	1535	rBV2	24059	26632	1.31%	0.148%
17	11.110	1547	1551	1554	rBV	624794	523713	25.82%	2.911%
18	11.657	1639	1644	1647	rBV2	74351	74815	3.69%	0.416%
19	12.316	1753	1756	1759	rBV	33412	32542	1.60%	0.181%
20	12.439	1774	1777	1781	rBV3	20611	26279	1.30%	0.146%
21	12.539	1788	1794	1796	rBV3	33598	51712	2.55%	0.287%
22	12.575	1796	1800	1804	rVV	98028	106570	5.26%	0.592%
23	12.610	1804	1806	1809	rVB2	25692	21421	1.06%	0.119%
24	12.692	1816	1820	1823	rBV	1181280	1032113	50.89%	5.736%
25	13.163	1897	1900	1902	rBV3	26764	30214	1.49%	0.168%
26	13.257	1912	1916	1919	rBV3	32579	36391	1.79%	0.202%
27	13.598	1972	1974	1980	rVB2	76158	80062	3.95%	0.445%
28	13.733	1993	1997	2000	rBV	565180	540074	26.63%	3.001%
29	14.233	2079	2082	2085	rBV3	28752	37540	1.85%	0.209%
30	14.380	2104	2107	2112	rBV	168800	152743	7.53%	0.849%
31	14.645	2150	2152	2155	rVB4	35999	35745	1.76%	0.199%
32	14.821	2180	2182	2184	rBV2	35171	36456	1.80%	0.203%
33	15.104	2226	2230	2235	rBV	455872	514979	25.39%	2.862%
34	15.539	2301	2304	2308	rBV2	37875	47710	2.35%	0.265%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

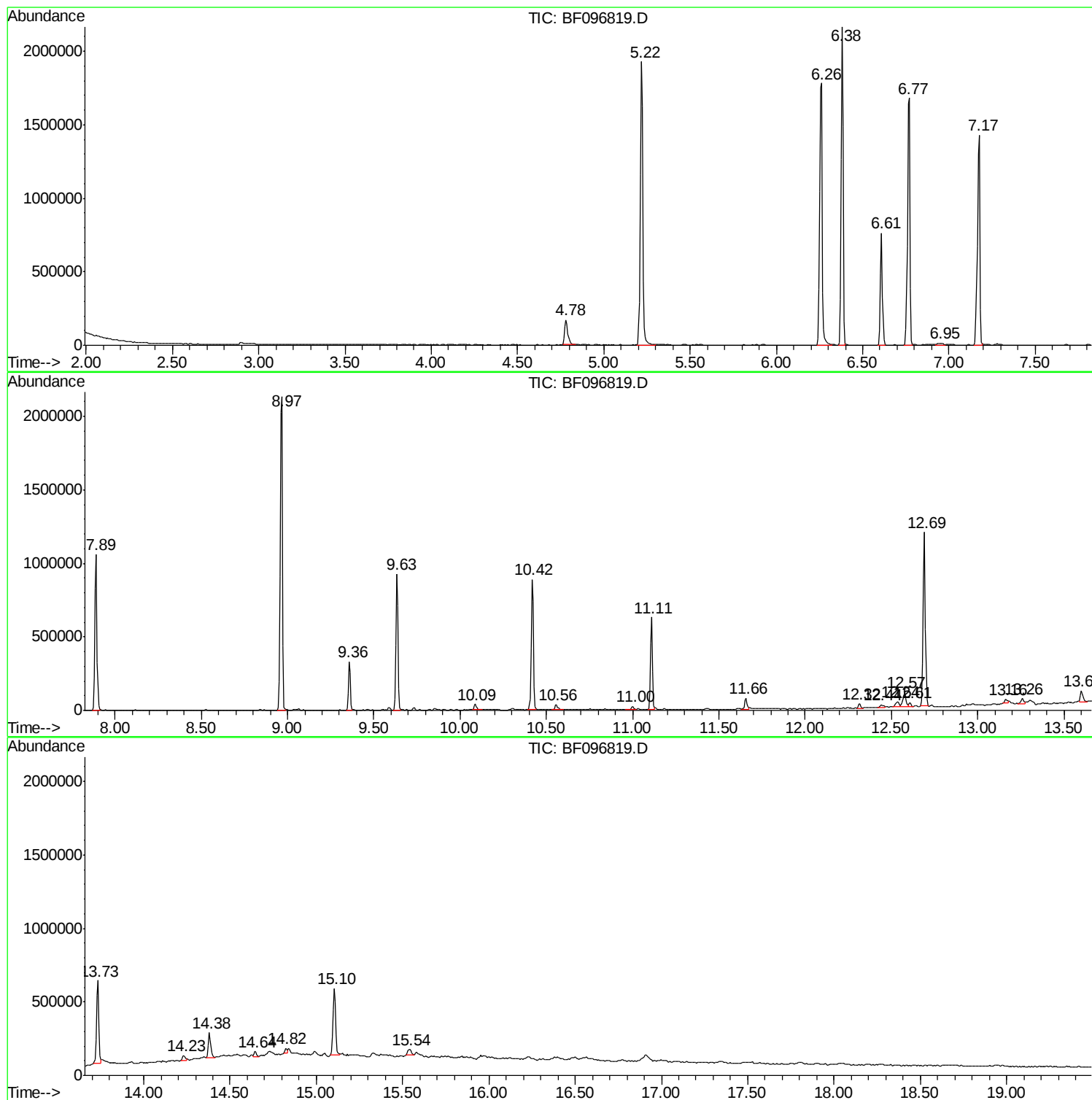
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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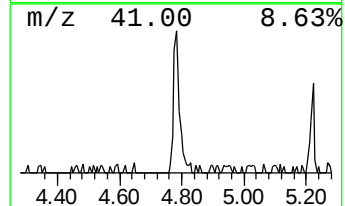
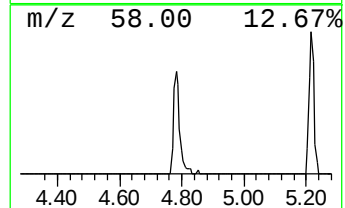
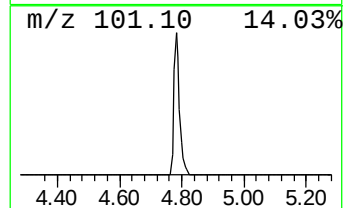
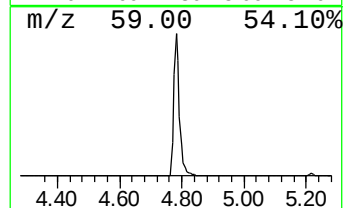
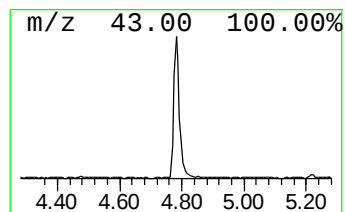
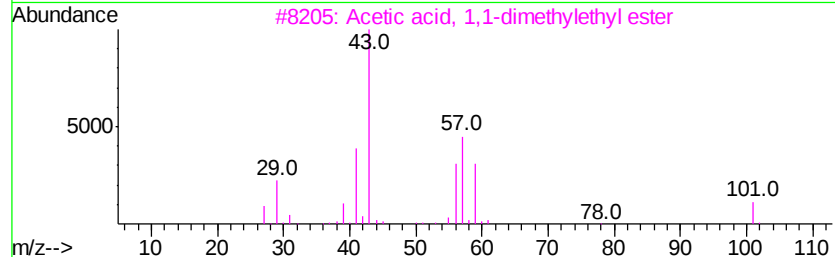
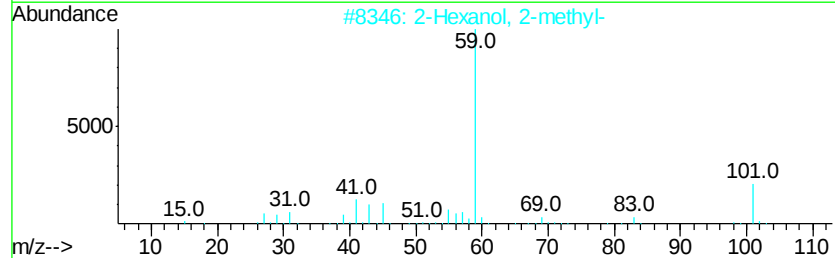
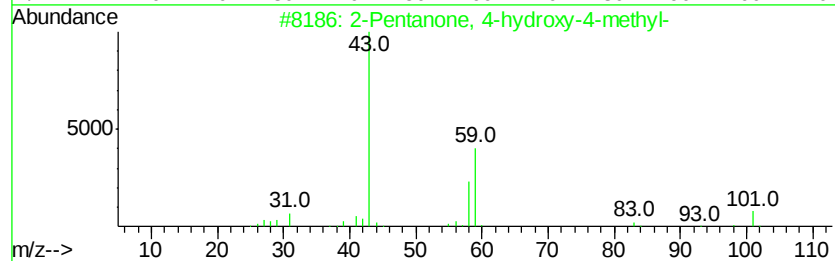
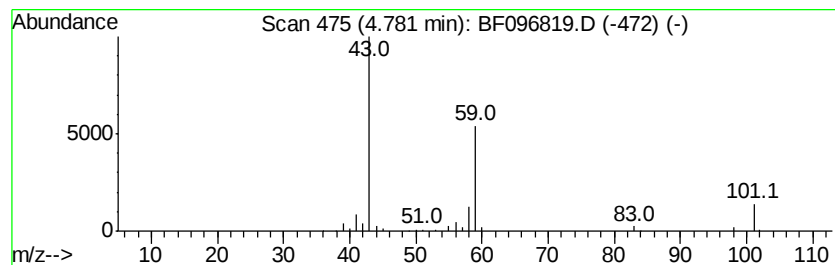
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	7.18 ng	217540	1,4-Dichlorobenzene-d4	6.61

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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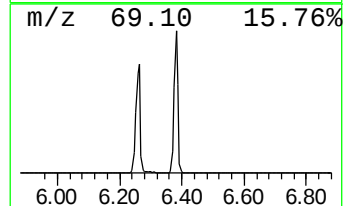
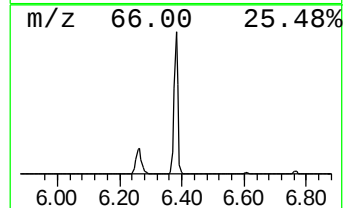
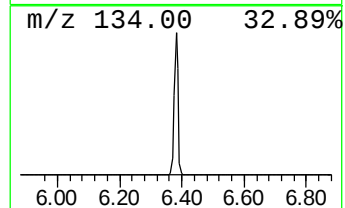
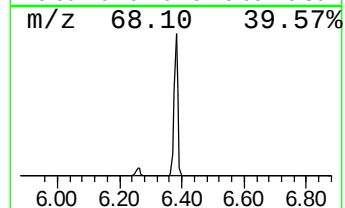
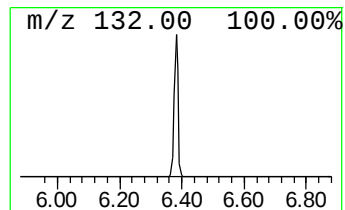
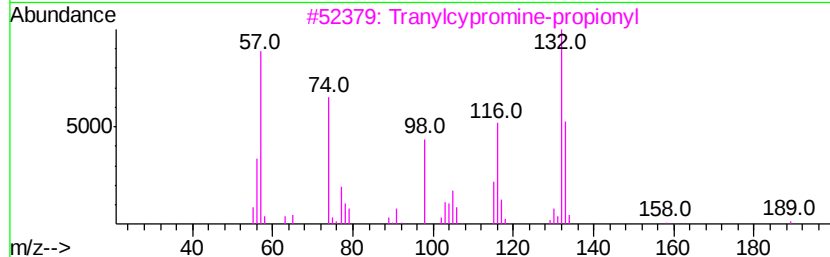
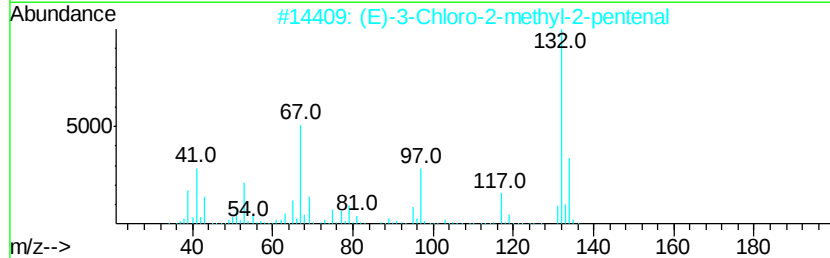
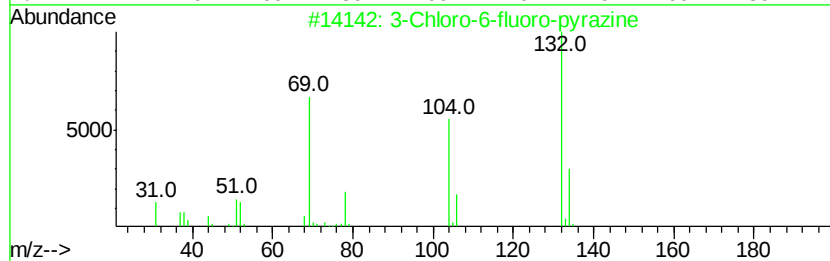
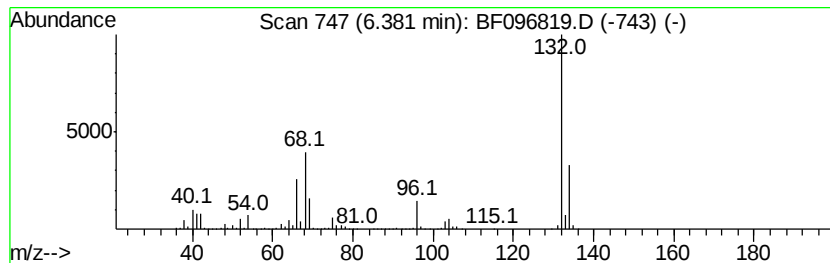
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.38	62.87 ng	1905280	1,4-Dichlorobenzene-d4	6.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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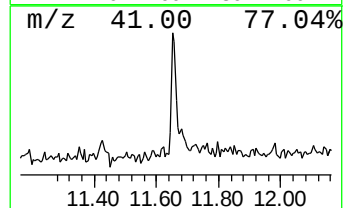
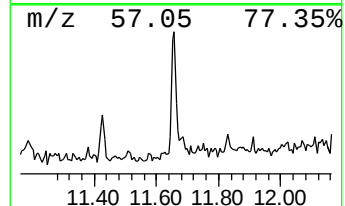
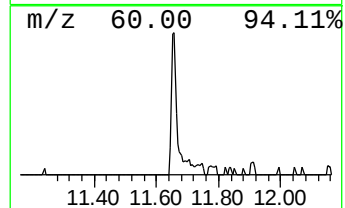
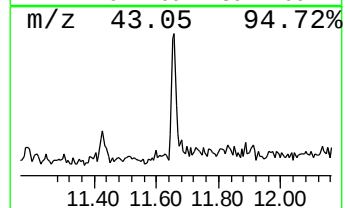
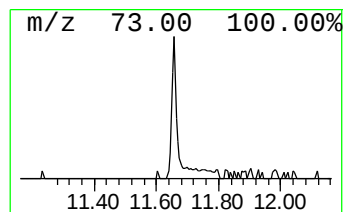
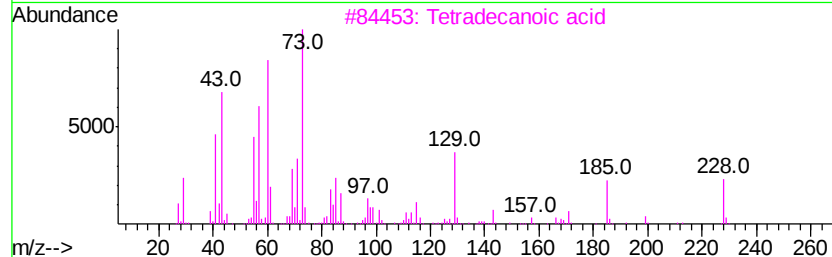
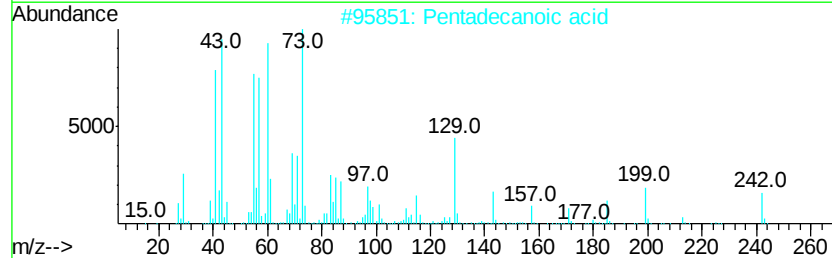
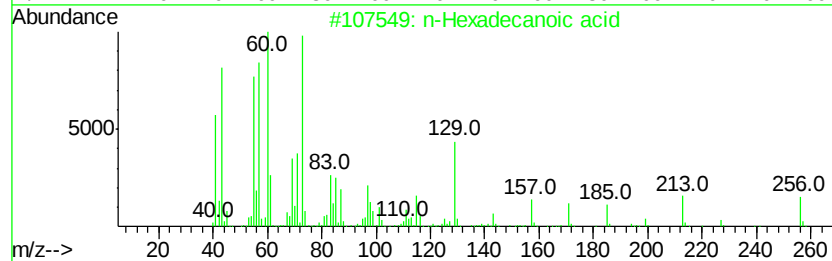
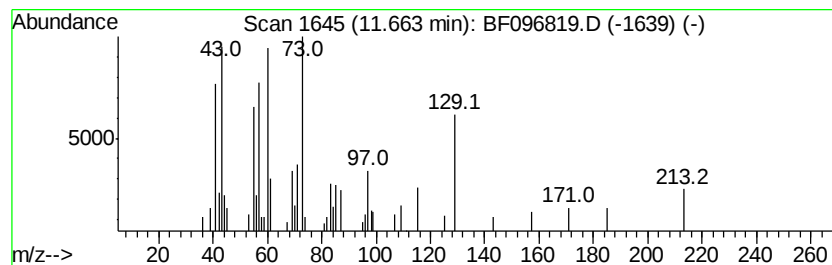
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	2.86 ng	74815	Phenanthrene-d10	11.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50



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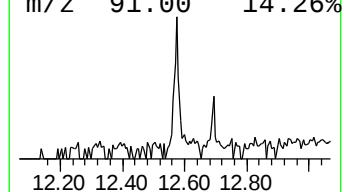
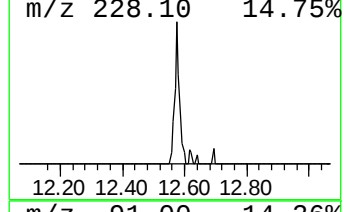
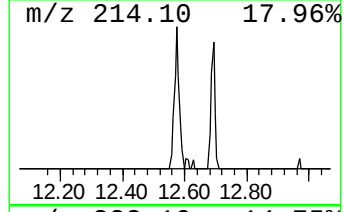
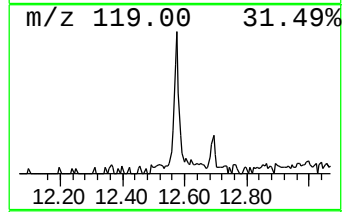
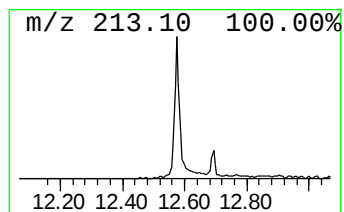
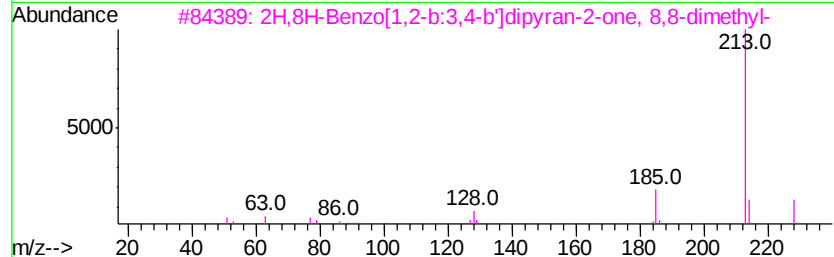
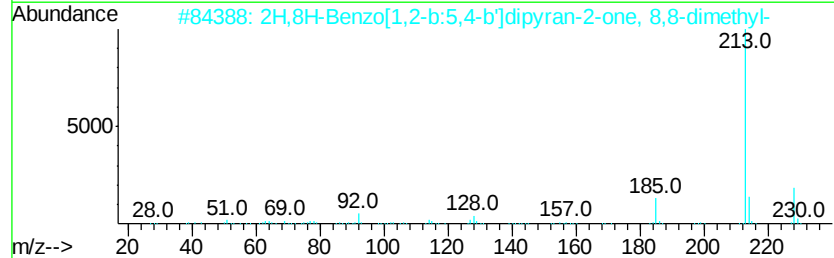
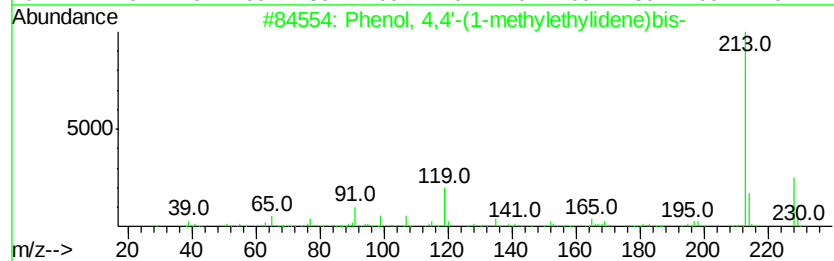
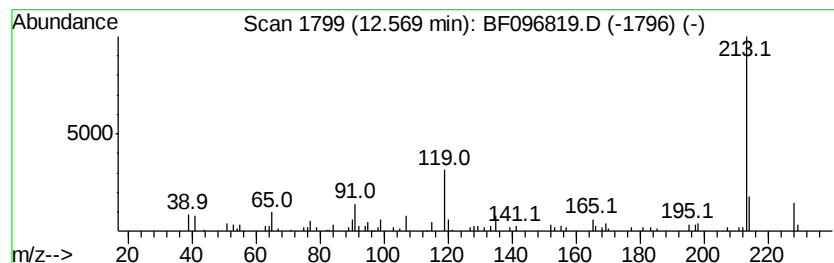
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.95 ng	106570	Chrysene-d12	13.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2		2H,8H-Benzo[1,2-b:5,4-b']dipyr...	228	C14H12O3	000553-19-5	58
3		2H,8H-Benzo[1,2-b:3,4-b']dipyr...	228	C14H12O3	000523-59-1	58
4		4-Adamantan-1-yl-2-(2-methylprop...	333	C19H27NO2S	1000311-66-6	50
5		Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50



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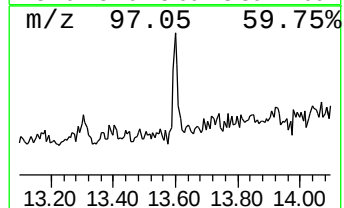
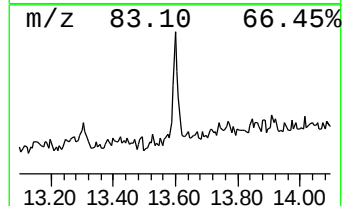
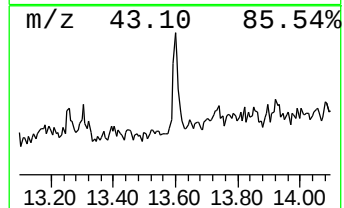
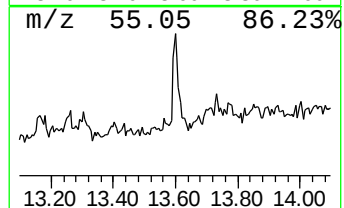
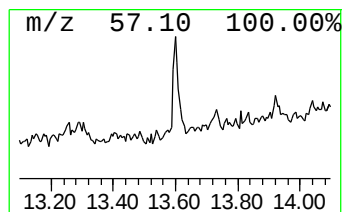
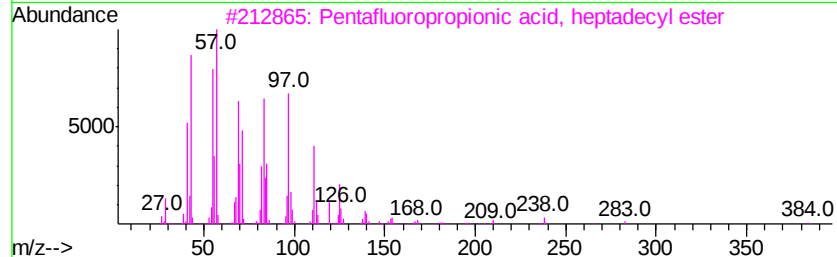
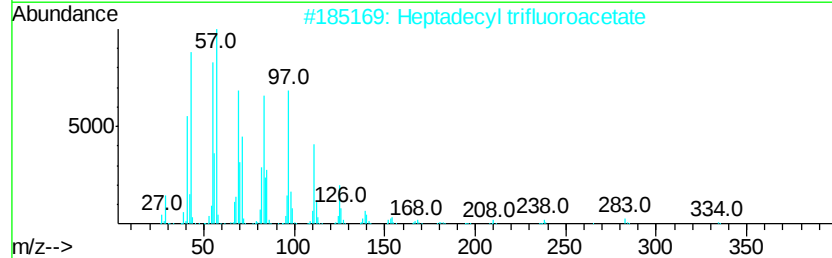
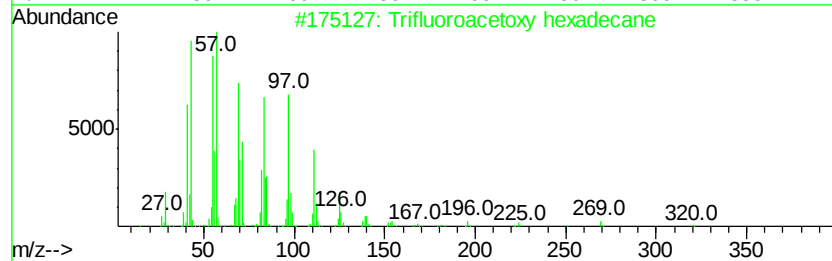
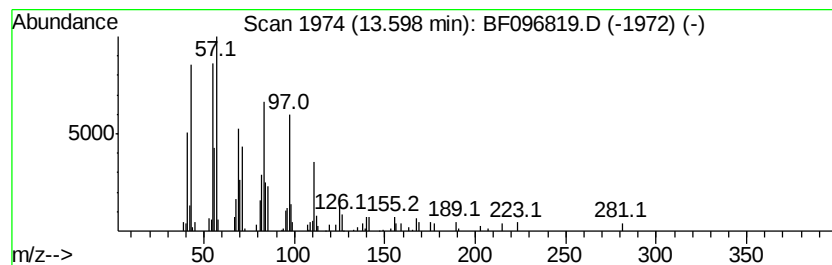
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	2.96 ng	80062	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071717\
Data File : BF096819.D
Acq On : 17 Jul 2017 15:09
Operator : SJ/JU
Sample : I4188-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1(0-10)COMP

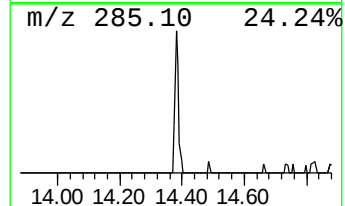
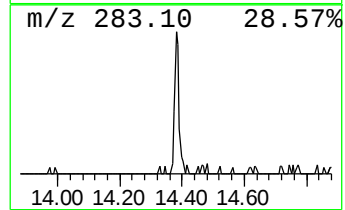
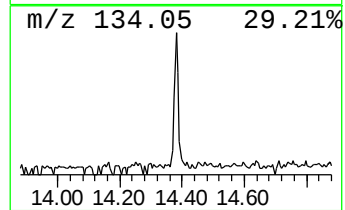
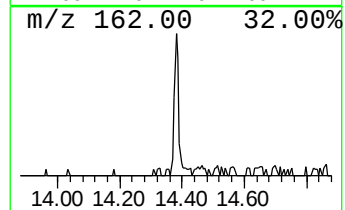
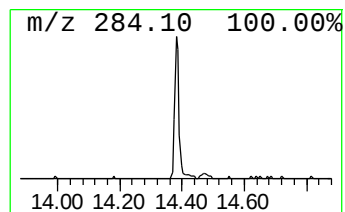
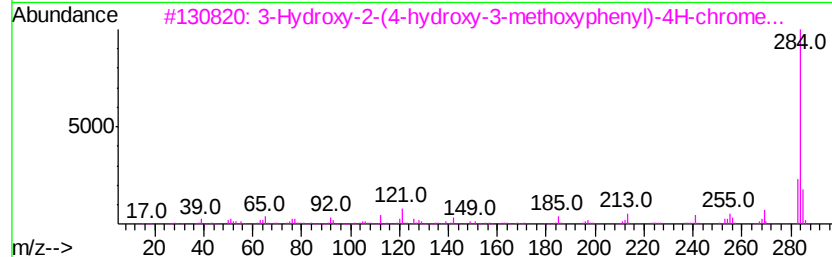
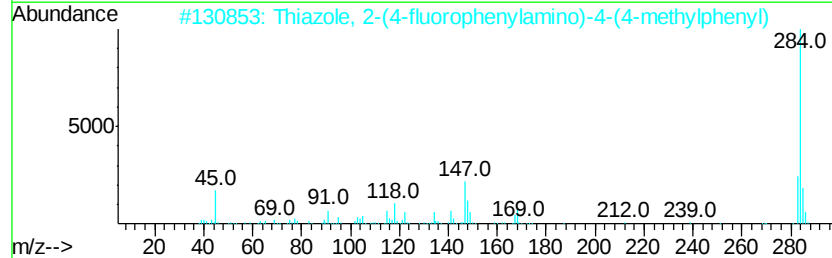
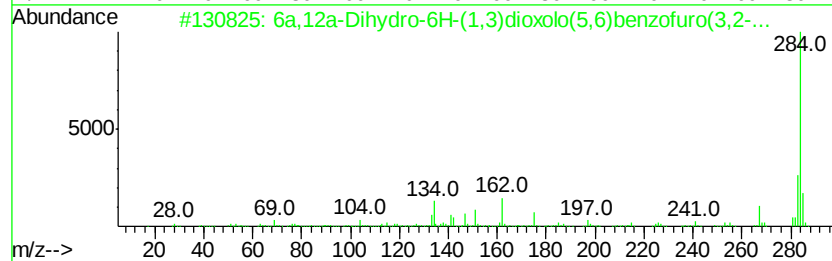
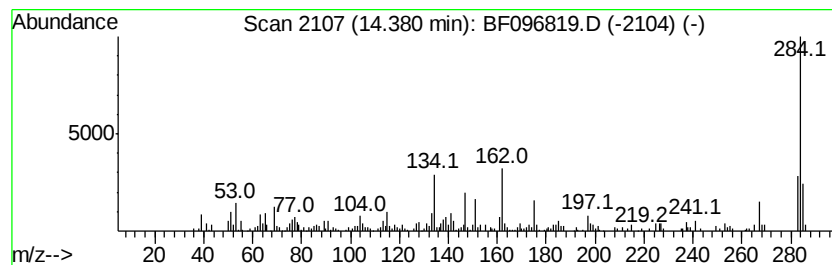
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	5.66 ng	152743	Chrysene-d12	13.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	94
2			Thiazole, 2-(4-fluorophenylamino...	284	C16H13FN2S	340801-58-3	70
3			3-Hydroxy-2-(4-hydroxy-3-methoxy...	284	C16H12O5	159184-95-9	53
4			Dibenz[a,c]cyclohexane, 2,4,7-tr...	284	C18H20O3	145068-33-3	50
5			Benzofuran-3-one, 2-[3-hydroxy-4...	284	C16H12O5	1000128-62-8	49



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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B1(0-10)COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.78	7.2	ng	217540	1	6.61	606083	20.0
unknown6.38	6.38	62.9	ng	1905280	1	6.61	606083	20.0
n-Hexadecanoic acid	11.66	2.9	ng	74815	4	11.11	523713	20.0
Phenol, 4,4'-(1-m...	12.57	4.0	ng	106570	5	13.73	540074	20.0
Trifluoroacetoxy ...	13.60	3.0	ng	80062	5	13.73	540074	20.0
6a,12a-Dihydro-6H...	14.38	5.7	ng	152743	5	13.73	540074	20.0