

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091015\
 Data File : BF081571.D
 Acq On : 10 Sep 2015 17:14
 Operator : UM/IZ
 Sample : G3497-02
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B3

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-BF090115.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	1.474	10	12	17	rBV	13497	34278	2.00%	0.225%
2	1.554	17	19	45	rVB	72801	236429	13.79%	1.552%
3	2.423	93	95	101	rBV	11387	20262	1.18%	0.133%
4	3.428	181	183	191	rBV	8543	22289	1.30%	0.146%
5	4.503	274	277	282	rBV	14701	29218	1.70%	0.192%
6	4.606	282	286	307	rVV	399181	1130041	65.90%	7.419%
7	5.440	356	359	376	rBV	873213	1626933	94.88%	10.682%
8	6.229	426	428	436	rBV	8631	17842	1.04%	0.117%
9	7.692	552	556	559	rBV	883211	1709813	99.72%	11.226%
10	7.783	561	564	573	rVB	1001490	1714667	100.00%	11.258%
11	8.263	603	606	612	rBB	207618	325655	18.99%	2.138%
12	8.595	631	635	638	rBV	670507	1198987	69.93%	7.872%
13	9.566	715	720	723	rBV	634529	1139420	66.45%	7.481%
14	11.155	856	859	863	rBV	238345	416647	24.30%	2.736%
15	13.807	1086	1091	1094	rBV	892986	1512315	88.20%	9.929%
16	14.870	1180	1184	1189	rBV	108127	177649	10.36%	1.166%
17	15.292	1217	1221	1226	rBB2	256552	435385	25.39%	2.859%
18	17.201	1384	1388	1391	rBV	552071	944608	55.09%	6.202%
19	17.841	1440	1444	1452	rBV	13180	31712	1.85%	0.208%
20	18.801	1525	1528	1532	rBV	258267	434569	25.34%	2.853%
21	18.927	1536	1539	1542	rBV	11430	20155	1.18%	0.132%
22	19.773	1609	1613	1616	rBV	14858	27015	1.58%	0.177%
23	19.956	1625	1629	1634	rBV2	10473	19357	1.13%	0.127%
24	20.561	1678	1682	1692	rBV	41478	96742	5.64%	0.635%
25	21.430	1755	1758	1760	rVB	23898	30041	1.75%	0.197%
26	21.819	1788	1792	1795	rBV2	11492	30294	1.77%	0.199%
27	21.933	1800	1802	1805	rBV2	18991	34305	2.00%	0.225%
28	22.139	1817	1820	1822	rBV	938537	1092774	63.73%	7.175%
29	22.573	1855	1858	1860	rBV	14423	18881	1.10%	0.124%
30	23.373	1926	1928	1929	rBV	61185	71244	4.15%	0.468%
31	23.407	1929	1931	1933	rVB	289788	292554	17.06%	1.921%
32	24.070	1984	1989	1993	rBV5	17088	39888	2.33%	0.262%
33	24.516	2025	2028	2031	rVB	13296	24569	1.43%	0.161%
34	24.756	2047	2049	2051	rBV	18766	25513	1.49%	0.168%

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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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35	24.802	2051	2053	2055	rVV	21983	20844	1.22%	0.137%
36	24.848	2055	2057	2060	rVV	182909	210351	12.27%	1.381%
37	26.219	2175	2177	2181	rBV2	10040	17668	1.03%	0.116%

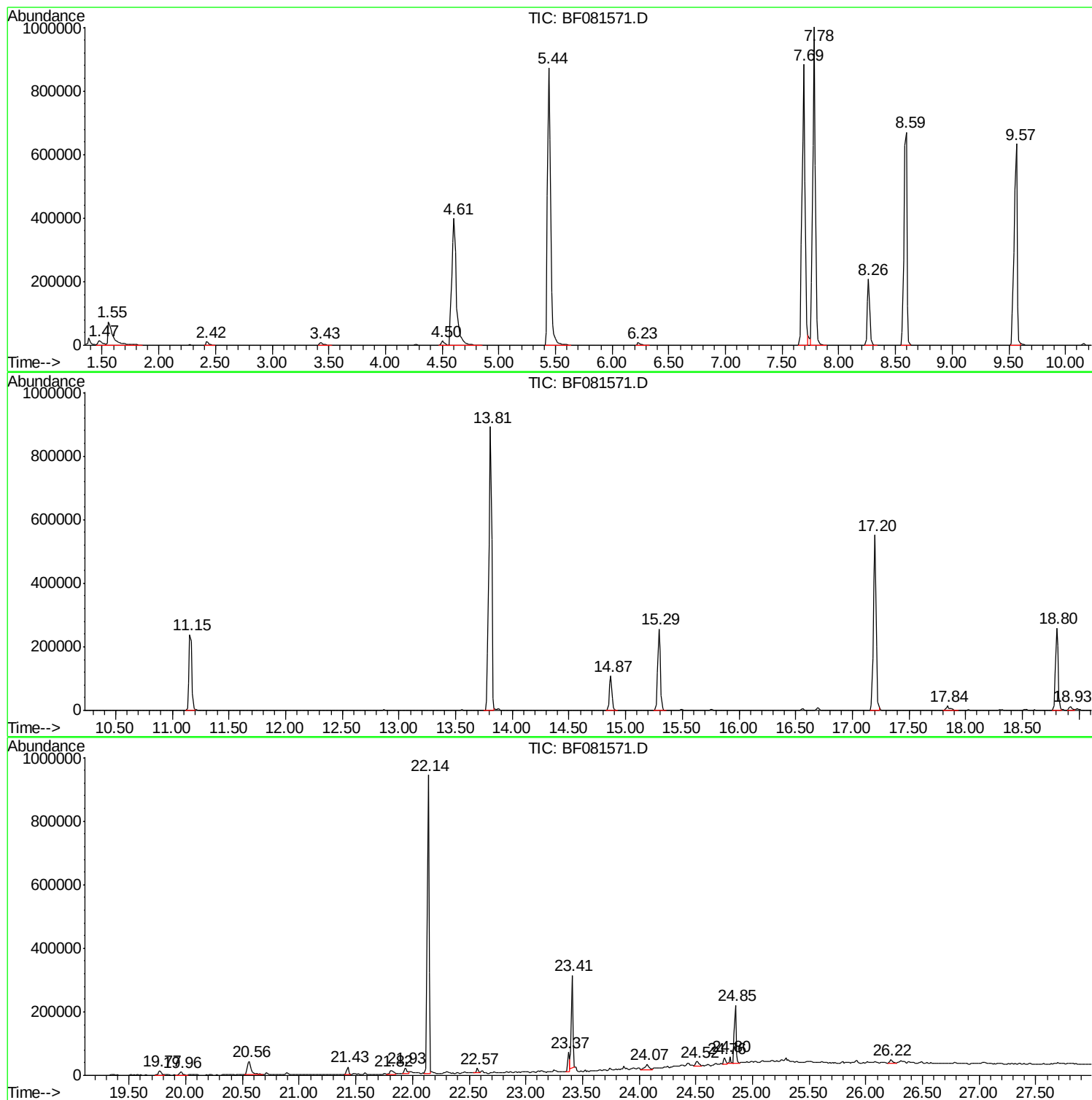
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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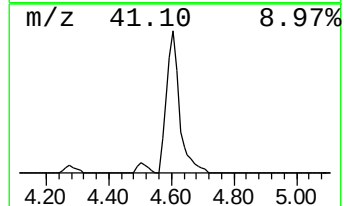
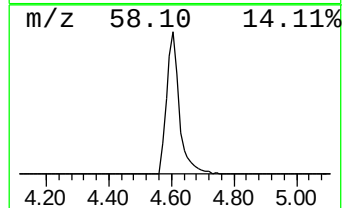
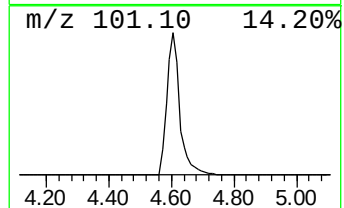
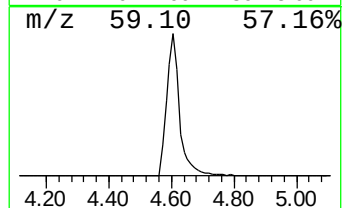
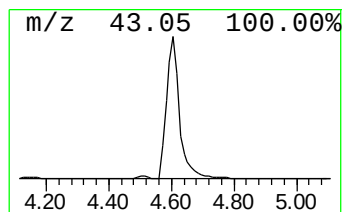
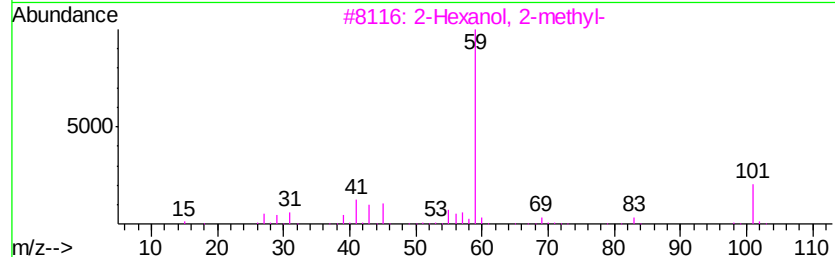
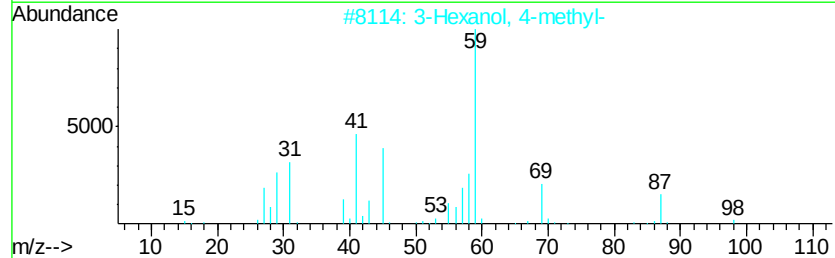
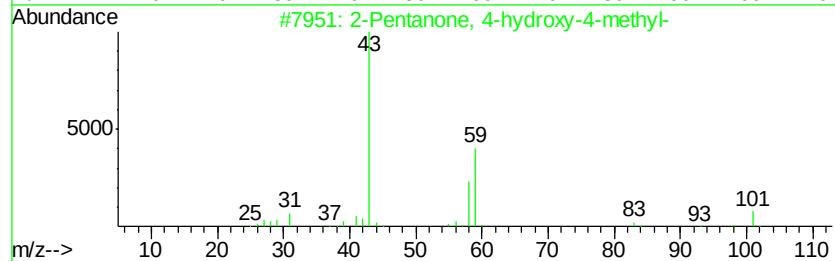
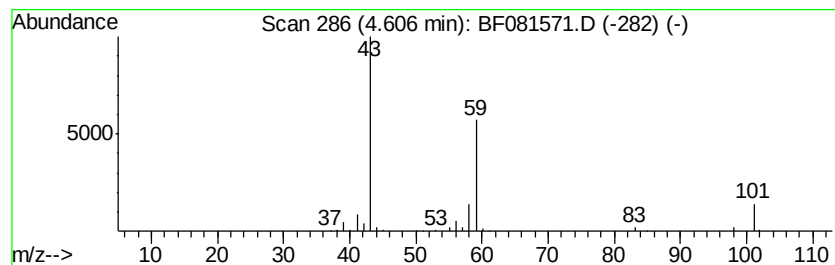
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.61	69.40 ng	1130040	1,4-Dichlorobenzene-d4	8.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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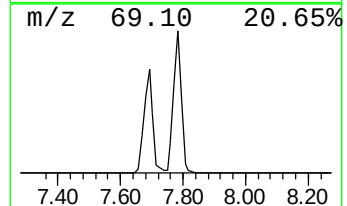
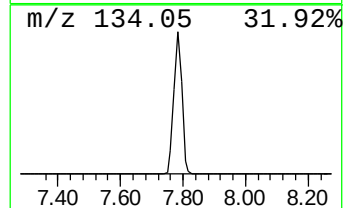
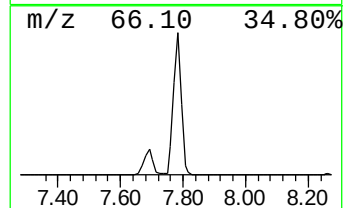
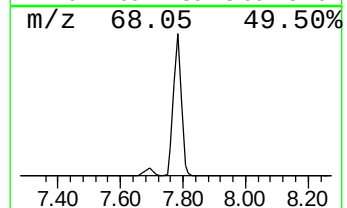
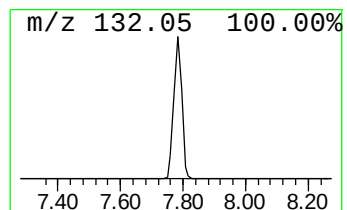
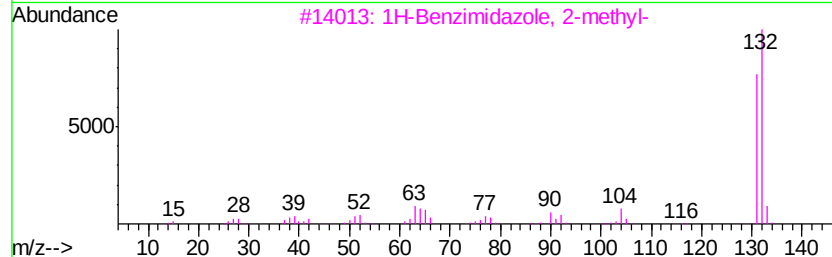
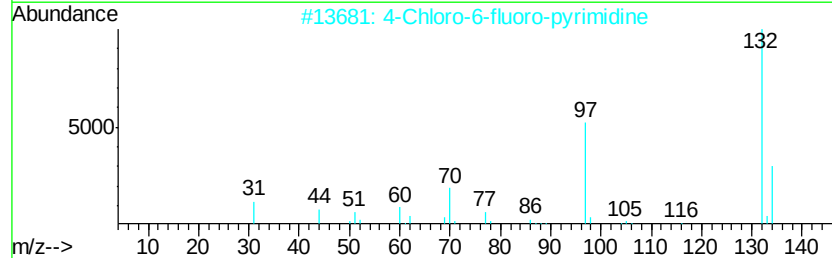
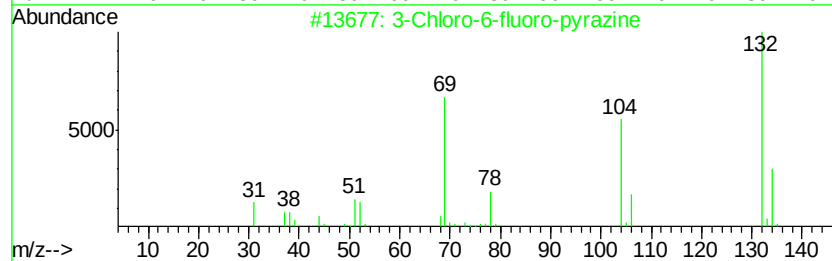
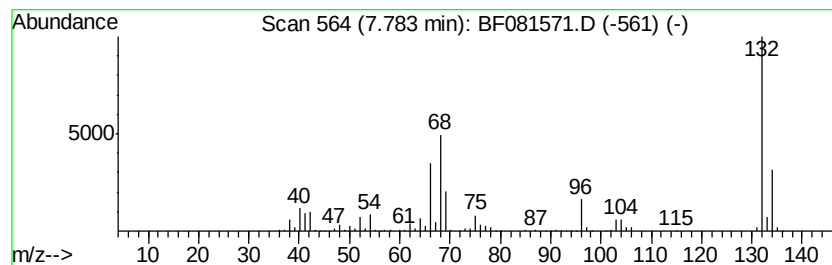
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.78 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.78	105.31 ng	1714670	1,4-Dichlorobenzene-d4	8.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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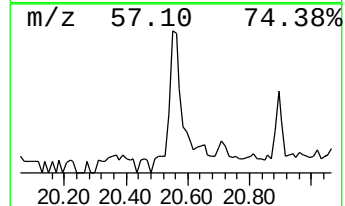
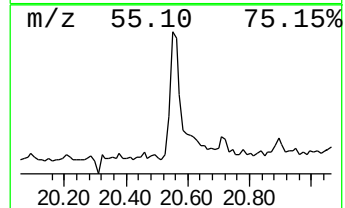
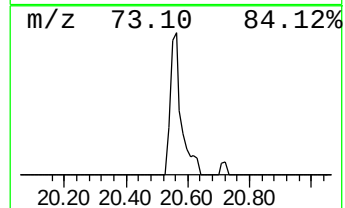
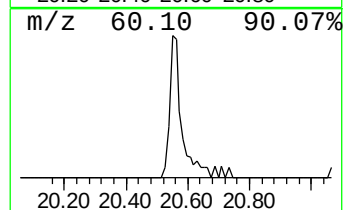
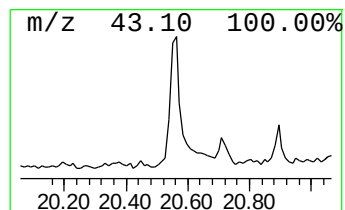
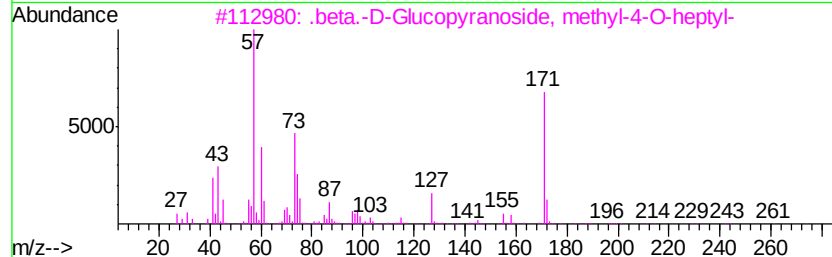
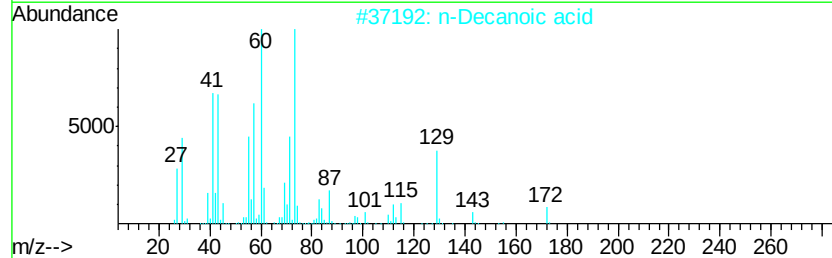
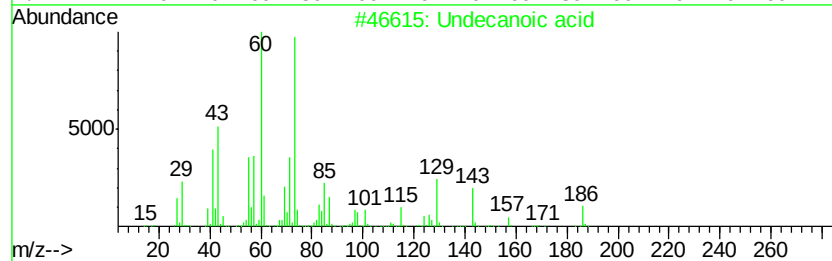
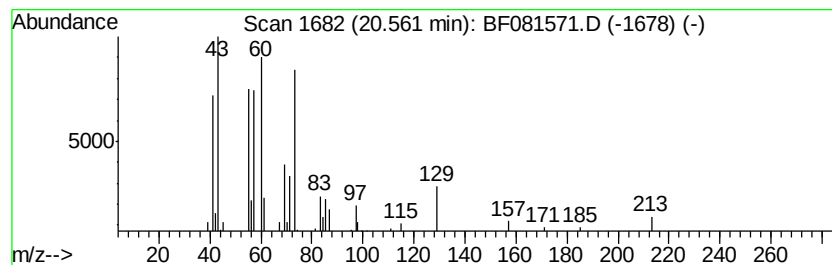
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Undecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.56	4.45 ng	96742	Phenanthrene-d10	18.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72	
2	n-Decanoic acid	172	C10H20O2	000334-48-5	50	
3	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	40	
4	Sedoheptulosan	192	C7H12O6	000469-90-9	38	
5	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	35	



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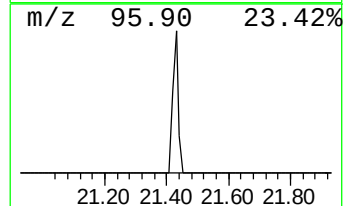
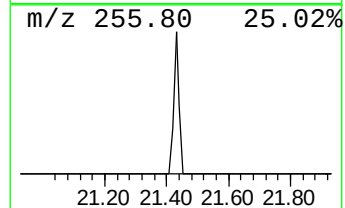
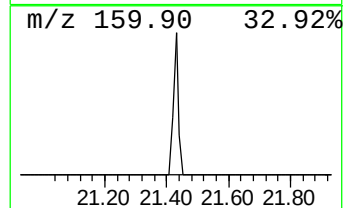
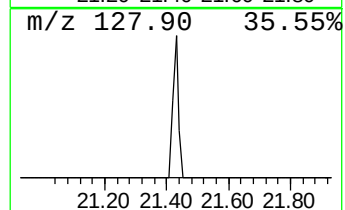
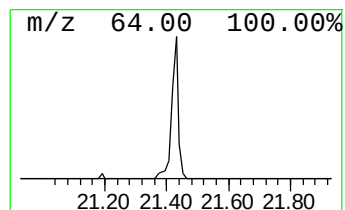
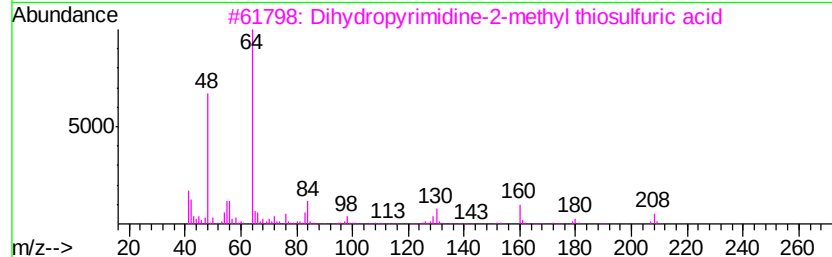
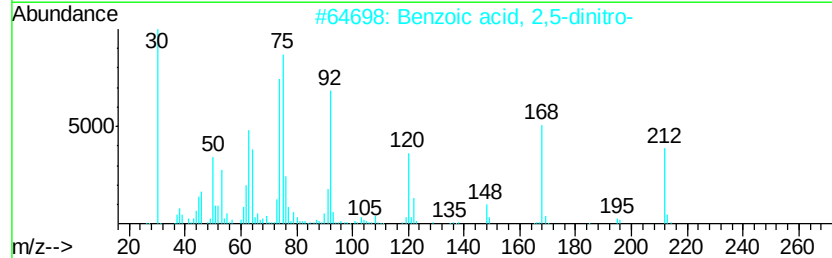
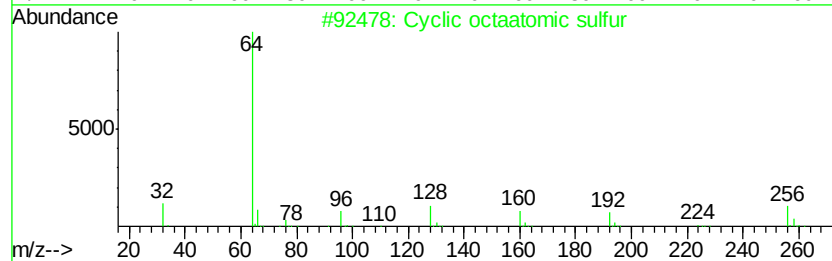
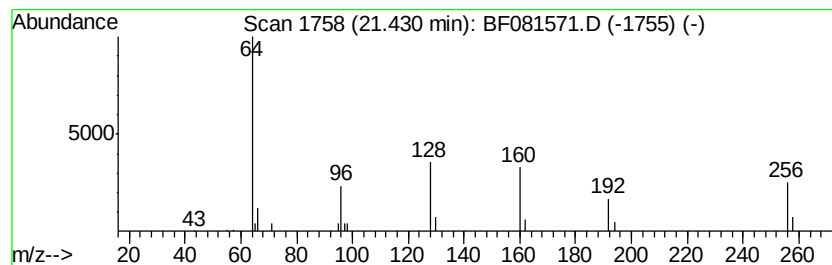
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclic octaatomic sulfur Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	2.05 ng	30041	Chrysene-d12	23.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	90
2		Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	53
3		Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	9
4		2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	9
5		1,2,5,6-Tetrathiocane	184	C4H8S4	001940-01-8	9



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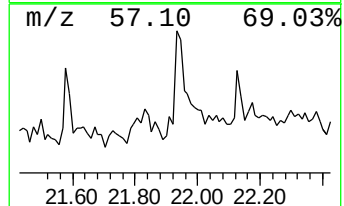
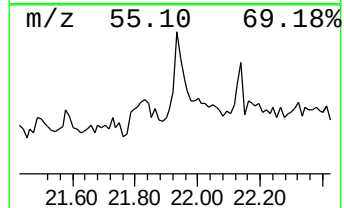
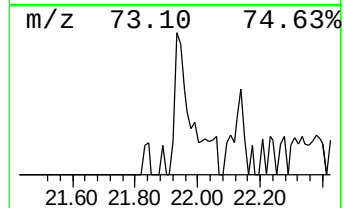
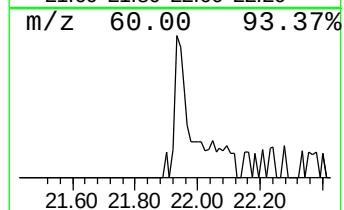
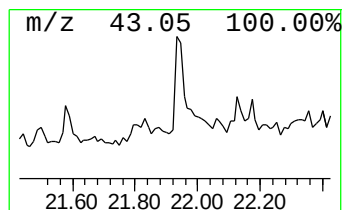
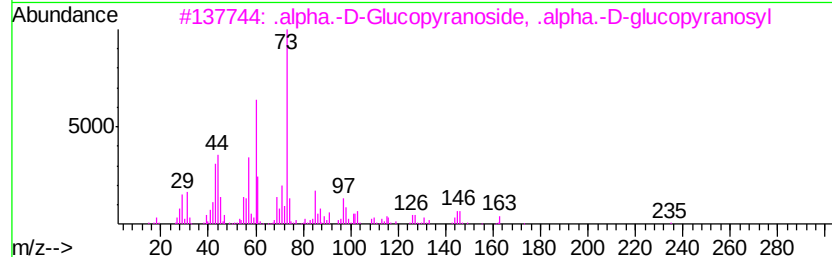
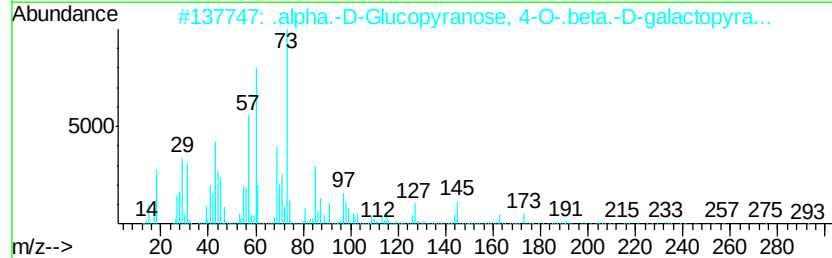
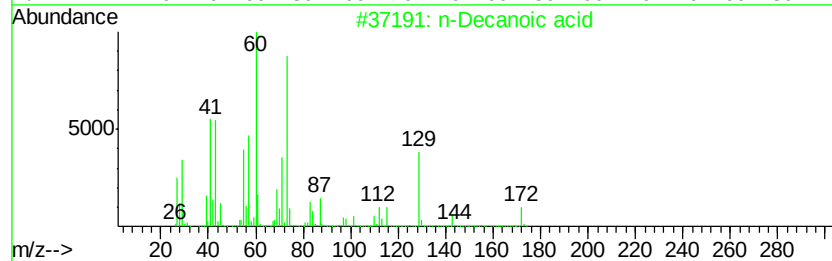
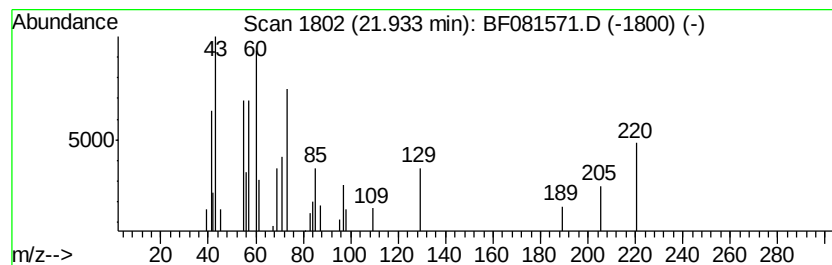
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 unknown21.93 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.93	2.35 ng	34305	Chrysene-d12	23.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Decanoic acid	172 C10H20O2	000334-48-5 43
2		.alpha.-D-Glucopyranose, 4-O-.be...	342 C12H22O11	014641-93-1 43
3		.alpha.-D-Glucopyranoside, .alph...	342 C12H22O11	000099-20-7 38
4		Lactose	342 C12H22O11	000063-42-3 38
5		.alpha.-D-Glucopyranoside, 0-.al...	504 C18H32O16	000597-12-6 27



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Misc :
ALS Vial : 4 Sample Multiplier: 1

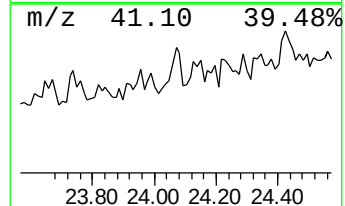
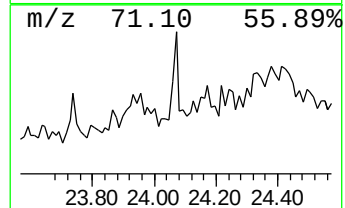
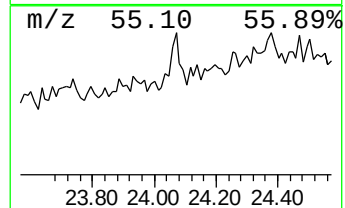
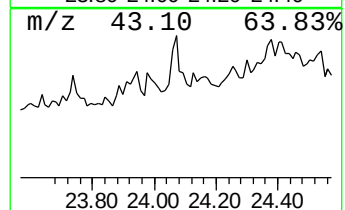
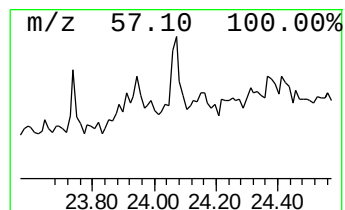
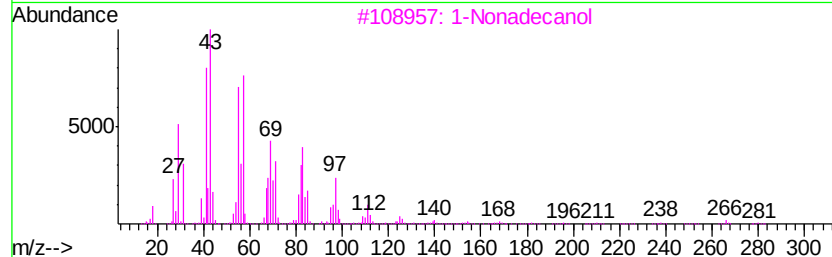
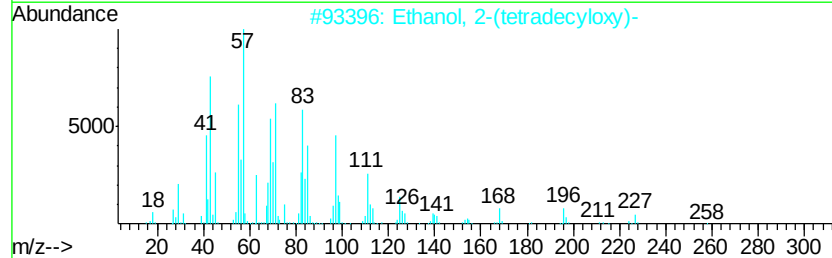
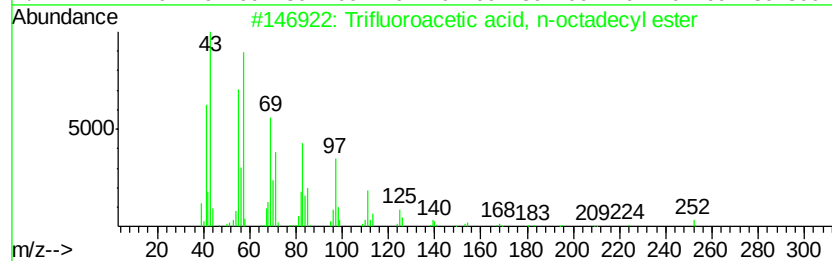
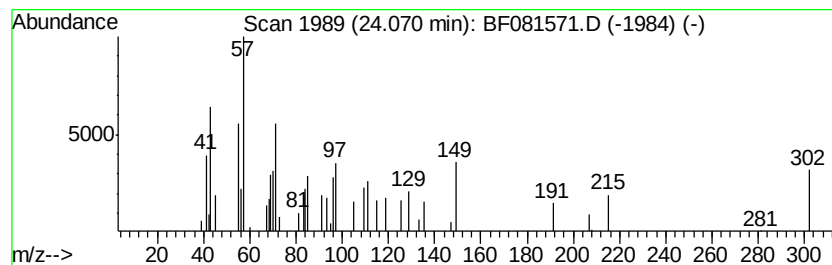
Instrument :
BNA_F
ClientSampleId :
B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown24.07 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.07	2.73 ng	39888	Chrysene-d12	23.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	27
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	27
3	1-Nonadecanol	284	C19H40O	001454-84-8	16
4	1-Heptadecanol	256	C17H36O	001454-85-9	16
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	16



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091015\
Data File : BF081571.D
Acq On : 10 Sep 2015 17:14
Operator : UM/IZ
Sample : G3497-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.61	69.4	ng	1130040	1	8.26	325655	20.0
unknown7.78	7.78	105.3	ng	1714670	1	8.26	325655	20.0
Undecanoic acid	20.56	4.5	ng	96742	4	18.80	434569	20.0
Cyclic octaatomic...	21.43	2.0	ng	30041	5	23.41	292554	20.0
unknown21.93	21.93	2.4	ng	34305	5	23.41	292554	20.0
unknown24.07	24.07	2.7	ng	39888	5	23.41	292554	20.0