

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062518\
 Data File : BF106783.D
 Acq On : 25 Jun 2018 20:36
 Operator : JU/SJ
 Sample : J3595-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SC-01-ABC

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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	5.207	484	488	497	rBB	81984	106645	7.39%	0.859%
2	5.601	551	555	559	rBV	1118113	1119310	77.54%	9.016%
3	6.601	720	725	728	rBV	1040068	1172907	81.25%	9.448%
4	6.737	743	748	751	rBV	1239125	1178997	81.67%	9.497%
5	6.954	782	785	789	rBB	356887	316438	21.92%	2.549%
6	7.113	808	812	815	rBV	1068275	975232	67.56%	7.855%
7	7.525	876	882	885	rBV	806126	784735	54.36%	6.321%
8	8.236	999	1003	1007	rBV	426640	402021	27.85%	3.238%
9	9.313	1181	1186	1189	rBV	1559435	1443557	100.00%	11.628%
10	9.701	1249	1252	1260	rVB	158258	144518	10.01%	1.164%
11	9.907	1284	1287	1290	rBV	29122	22052	1.53%	0.178%
12	10.001	1298	1303	1309	rVB	484009	478783	33.17%	3.857%
13	10.407	1370	1372	1375	rVB	53065	36921	2.56%	0.297%
14	10.625	1403	1409	1412	rBV	16454	20011	1.39%	0.161%
15	10.795	1433	1438	1441	rBV	975057	939662	65.09%	7.569%
16	10.883	1450	1453	1458	rBV	41925	48961	3.39%	0.394%
17	11.330	1525	1529	1531	rBV	26679	21235	1.47%	0.171%
18	11.489	1552	1556	1559	rBV	574529	496919	34.42%	4.003%
19	11.513	1559	1560	1564	rVB	38355	22465	1.56%	0.181%
20	12.707	1758	1763	1766	rBV	98807	83672	5.80%	0.674%
21	12.936	1795	1802	1808	rBV	80393	90550	6.27%	0.729%
22	13.077	1821	1826	1829	rBV	1458184	1417018	98.16%	11.414%
23	13.948	1970	1974	1978	rBV2	53239	60151	4.17%	0.485%
24	14.142	2002	2007	2010	rBV	393411	397696	27.55%	3.203%
25	14.166	2010	2011	2016	rVB	33449	19712	1.37%	0.159%
26	14.665	2093	2096	2101	rVB	38305	41704	2.89%	0.336%
27	14.989	2147	2151	2155	rVB	33690	34540	2.39%	0.278%
28	15.218	2186	2190	2193	rBV	29879	42725	2.96%	0.344%
29	15.542	2241	2245	2252	rVB	20471	28489	1.97%	0.229%
30	15.607	2252	2256	2262	rBV	27627	38972	2.70%	0.314%
31	15.677	2262	2268	2273	rBV	293990	384308	26.62%	3.096%
32	16.124	2339	2344	2350	rBV6	7789	15082	1.04%	0.121%
33	17.236	2528	2533	2540	rBV3	12333	28968	2.01%	0.233%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

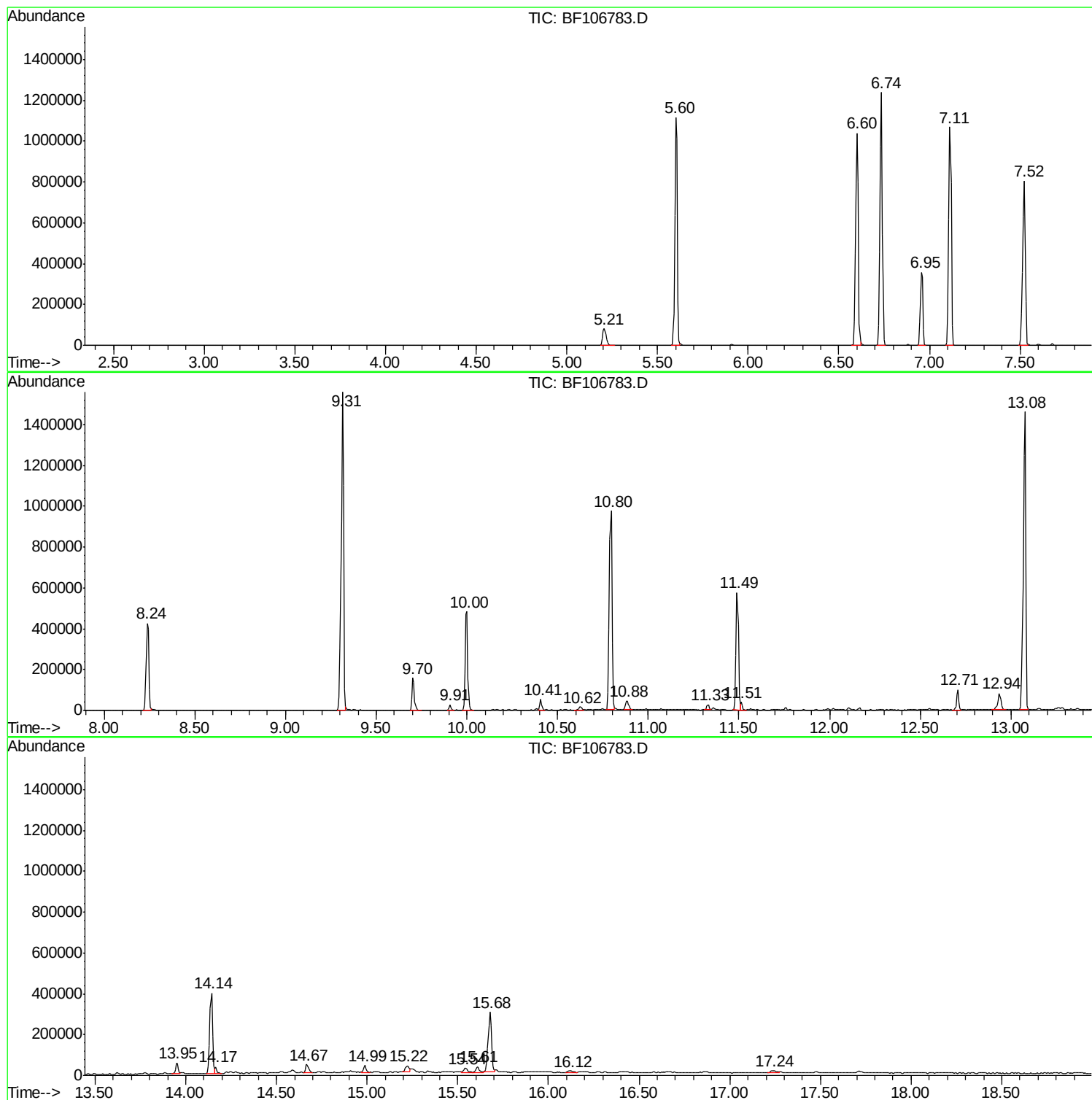
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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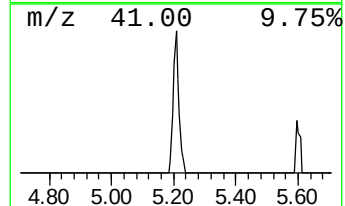
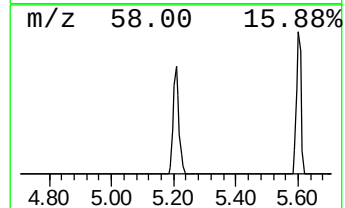
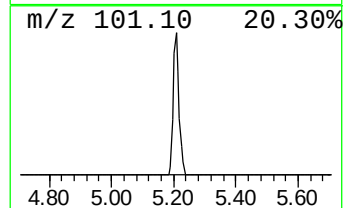
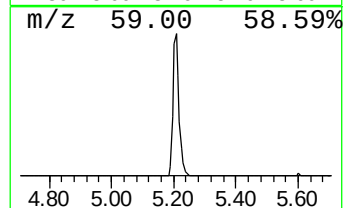
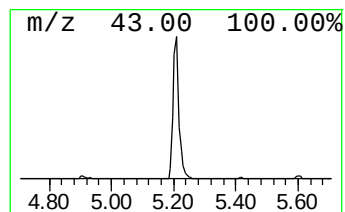
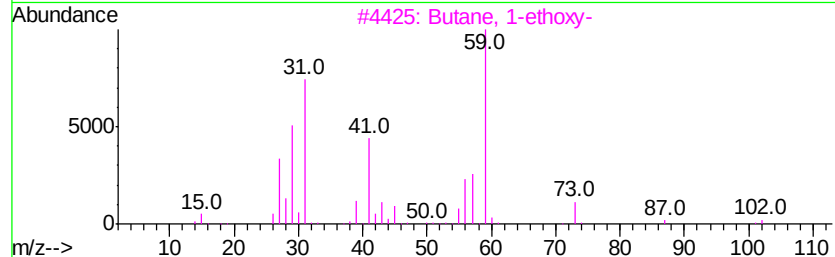
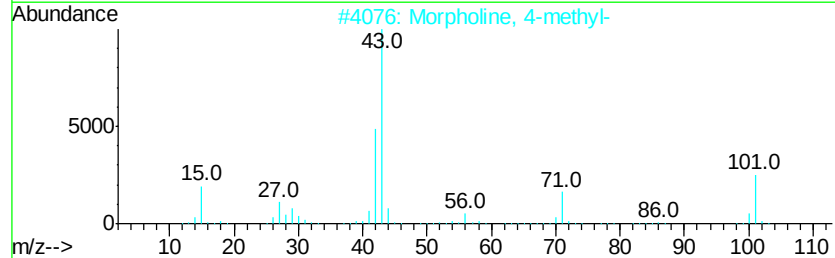
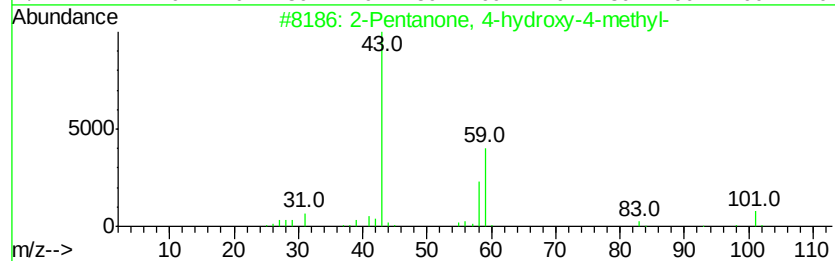
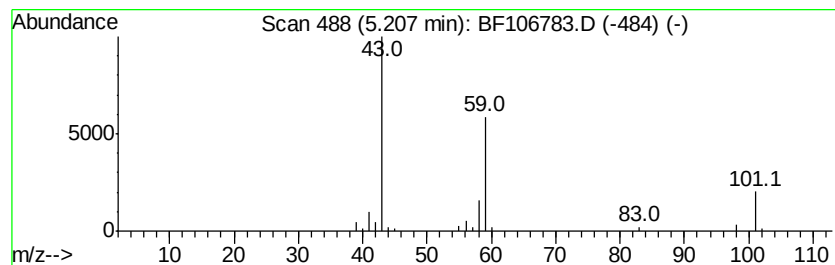
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	6.74 ng	106645	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4			Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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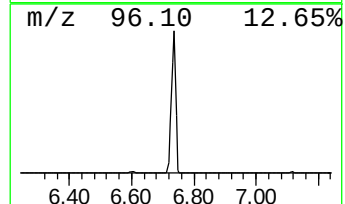
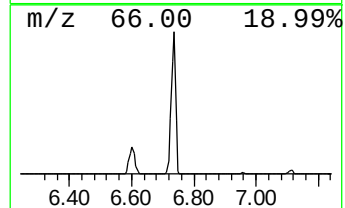
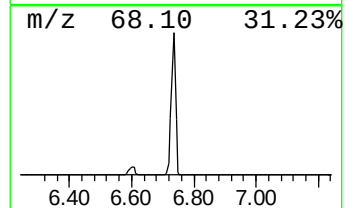
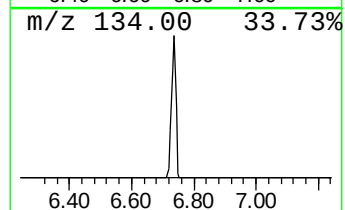
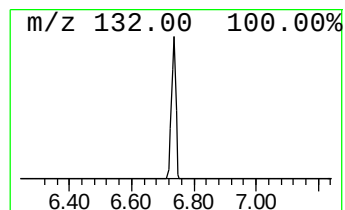
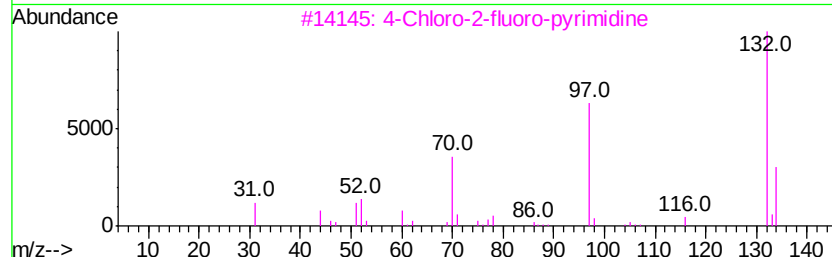
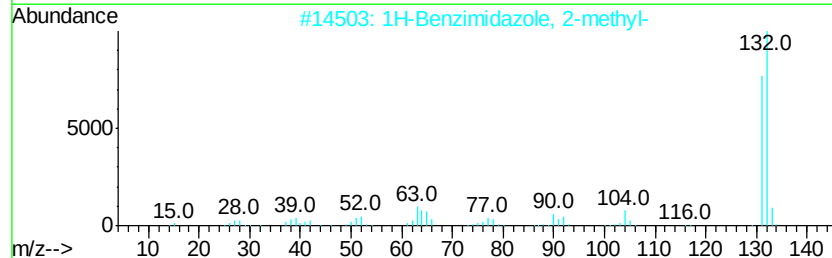
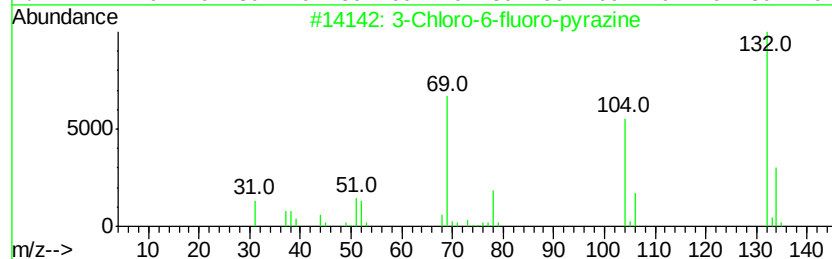
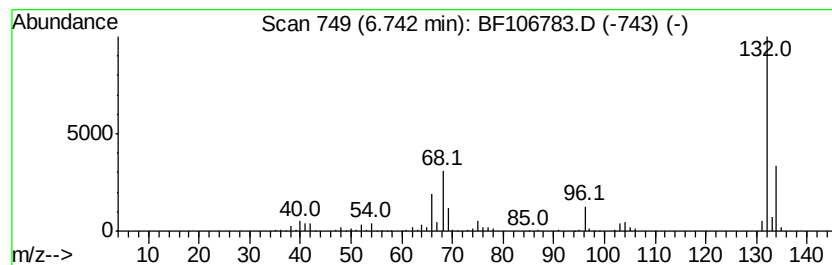
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	74.52 ng	1179000	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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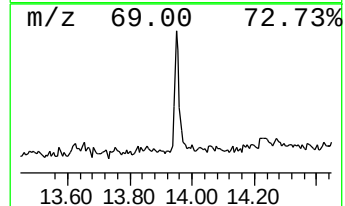
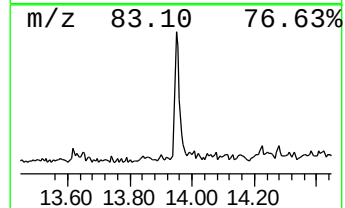
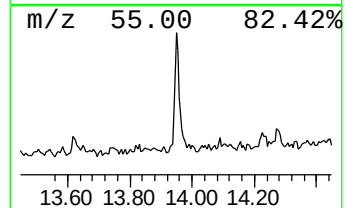
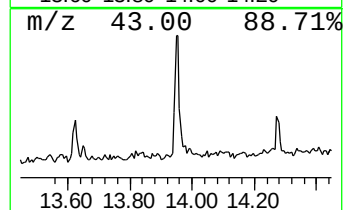
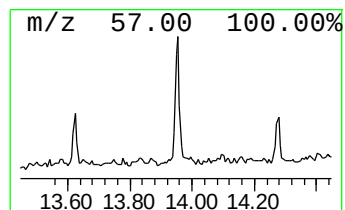
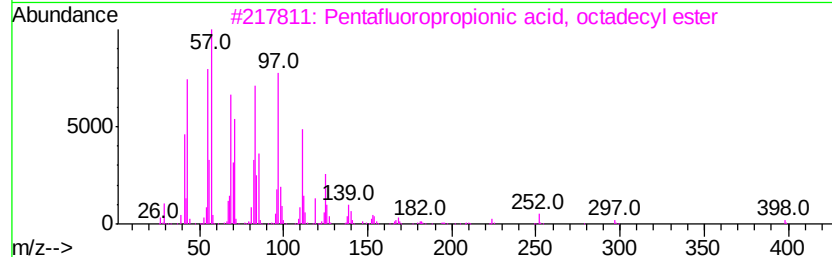
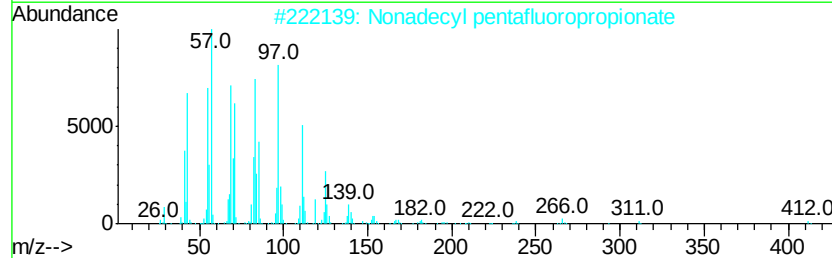
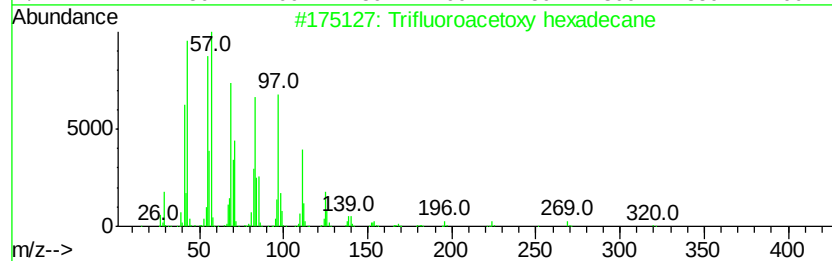
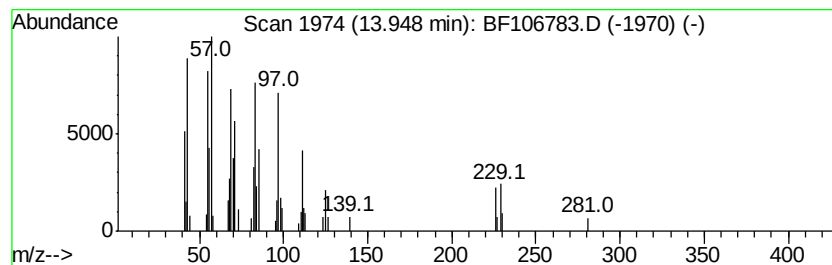
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.02 ng	60151	Chrysene-d12	14.14

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	959261-25-7	87
4		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	87
5		Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87



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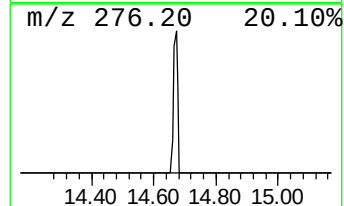
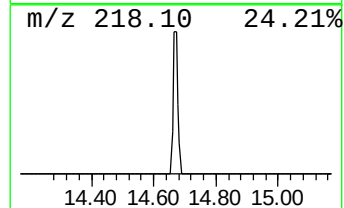
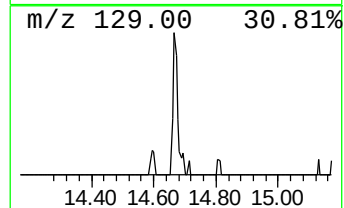
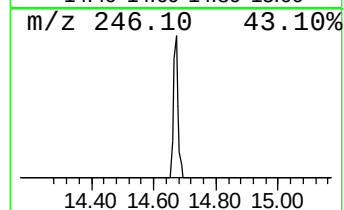
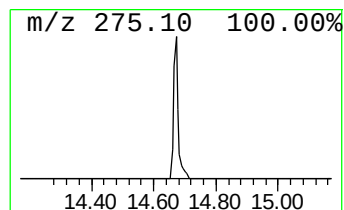
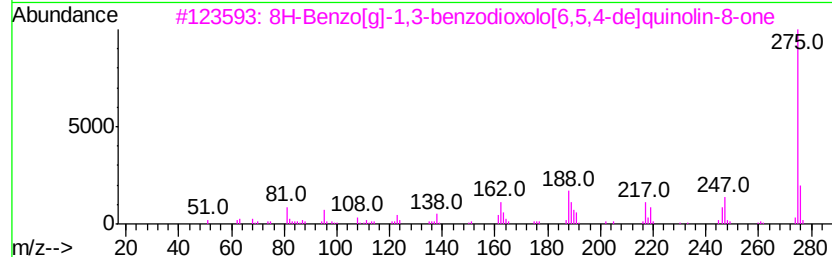
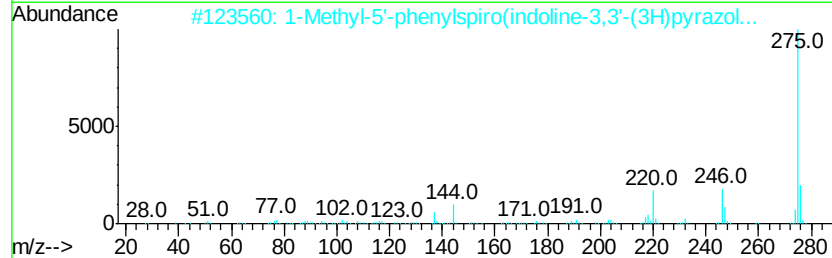
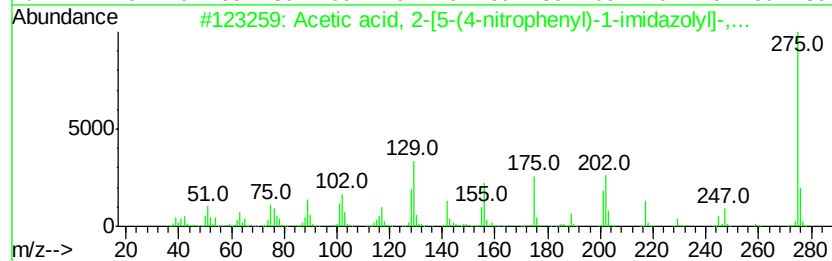
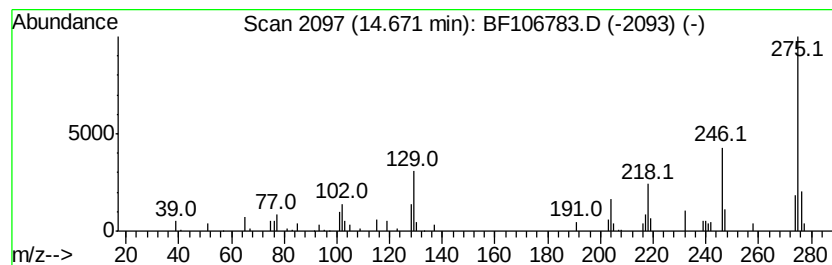
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Acetic acid, 2-[5-(4-nitrop... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	2.10 ng	41704	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-[5-(4-nitrophenyl...	275	C13H13N3O4	351064-45-4	58	
2	1-Methyl-5'-phenylspiro(indoline...	275	C17H13N3O	015970-21-5	43	
3	8H-Benzo[a]-1,3-benzodioxolo[6,5...	275	C17H9NO3	000475-75-2	38	
4	3,5-Diamino-6-[3,4-diethoxypheny...	275	C13H17N5O2	058848-69-4	37	
5	Naphthalen-1-yl amine, N-(benzo[...	275	C18H13NO2	202599-86-8	35	



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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...	5.21	6.7	ng	106645	1	6.95	316438	20.0
unknown6.74	6.74	74.5	ng	1179000	1	6.95	316438	20.0
Trifluoroacetoxy ...	13.95	3.0	ng	60151	5	14.14	397696	20.0
Acetic acid, 2-[5...	14.67	2.1	ng	41704	5	14.14	397696	20.0