

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096559.D
 Acq On : 7 Jul 2017 15:15
 Operator : SJ/MA
 Sample : I4064-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF004-01

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	471	476	487	rVB	476526	621237	20.95%	2.510%
2	5.310	543	548	551	rBV	2777293	2830308	95.44%	11.436%
3	6.340	717	723	733	rVB	2669483	2965606	100.00%	11.983%
4	6.469	740	745	748	rBV	2818523	2800837	94.44%	11.317%
5	6.693	780	783	787	rBV	788528	698062	23.54%	2.821%
6	6.851	806	810	814	rBV	2148945	1956376	65.97%	7.905%
7	7.257	873	879	882	rBV	1868175	1827035	61.61%	7.382%
8	7.975	997	1001	1005	rBV	932565	854947	28.83%	3.454%
9	9.057	1179	1185	1188	rBV	2736089	2615996	88.21%	10.570%
10	9.445	1247	1251	1255	rBV	256178	205100	6.92%	0.829%
11	9.728	1294	1299	1303	rBV	1058227	912733	30.78%	3.688%
12	10.175	1372	1375	1378	rVB	54390	41272	1.39%	0.167%
13	10.516	1428	1433	1436	rBV	1558290	1550726	52.29%	6.266%
14	10.645	1451	1455	1463	rBV	60232	60499	2.04%	0.244%
15	11.204	1546	1550	1554	rBV	965838	875712	29.53%	3.538%
16	12.792	1815	1820	1823	rBV	2295364	2228468	75.14%	9.004%
17	13.692	1969	1973	1983	rBV	150677	164354	5.54%	0.664%
18	13.833	1993	1997	2001	rBV	776956	650437	21.93%	2.628%
19	14.592	2122	2126	2138	rBV	331215	330522	11.15%	1.335%
20	14.686	2139	2142	2146	rVB	45024	46024	1.55%	0.186%
21	15.233	2230	2235	2241	rBV	431130	512753	17.29%	2.072%

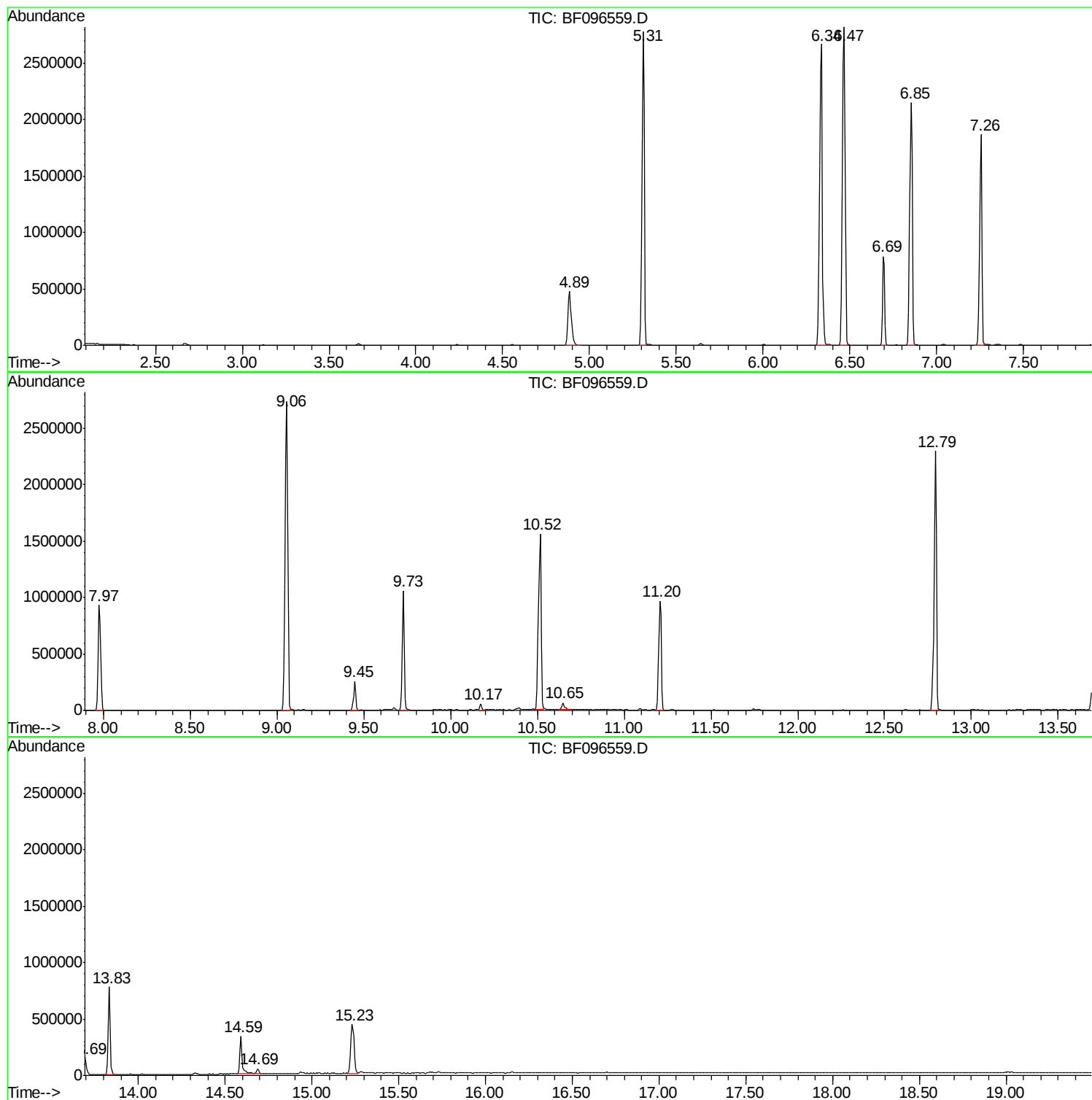
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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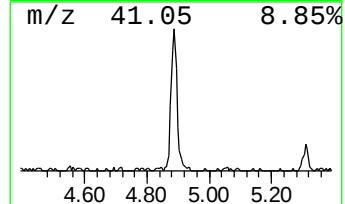
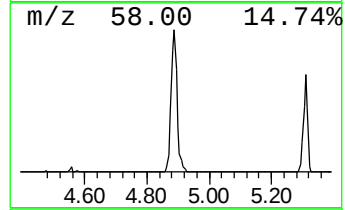
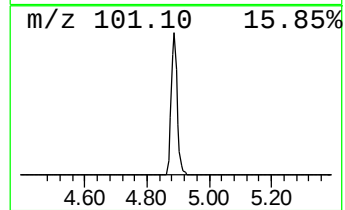
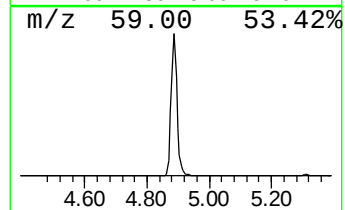
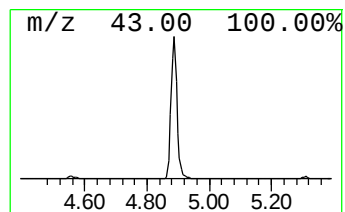
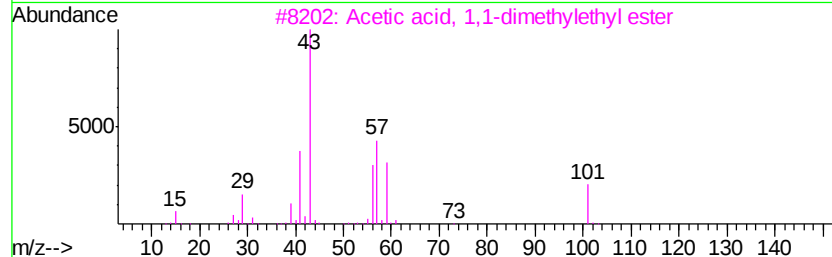
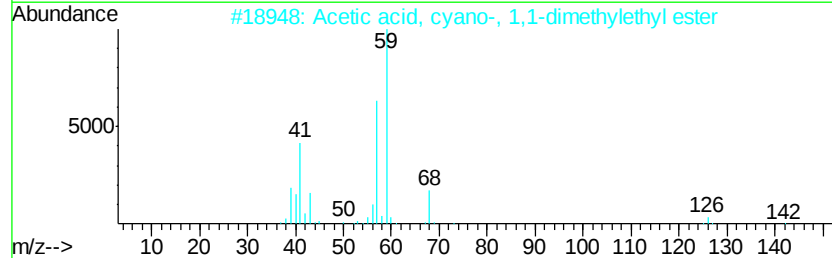
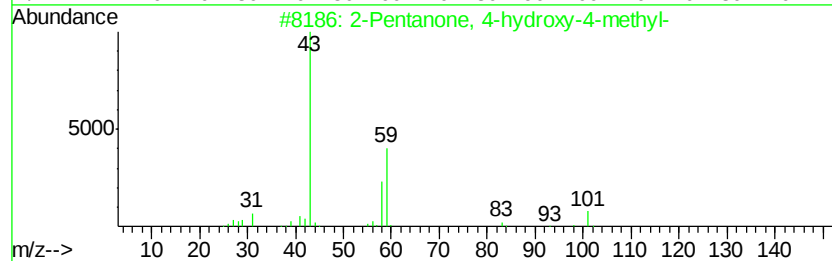
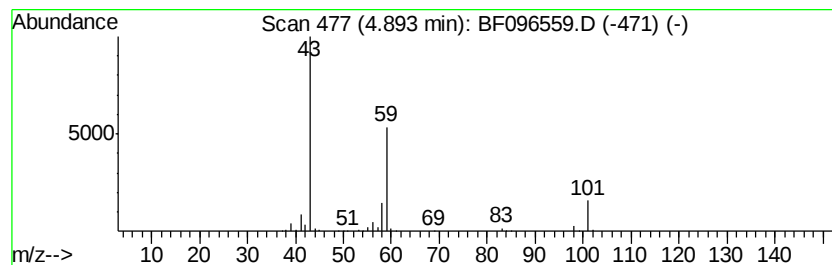
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	17.80 ng	621237	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	38
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			3-Hexanol	102	C6H14O	000623-37-0	9
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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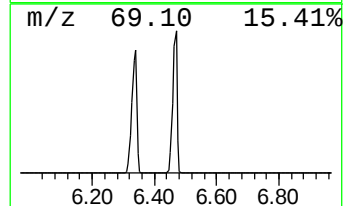
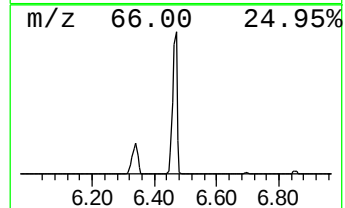
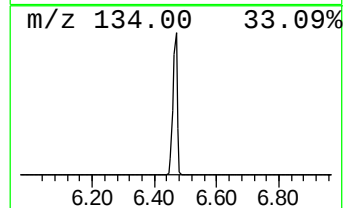
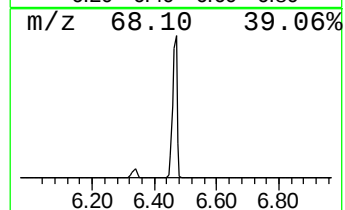
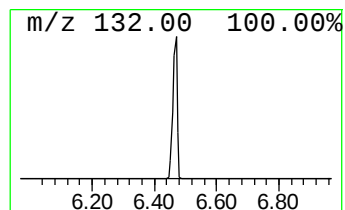
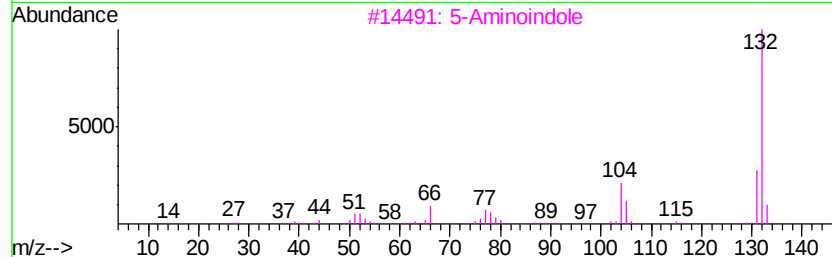
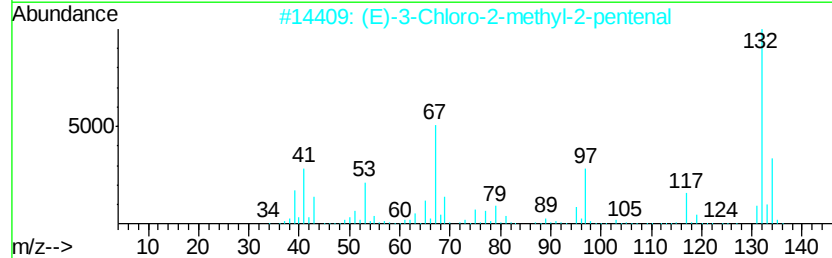
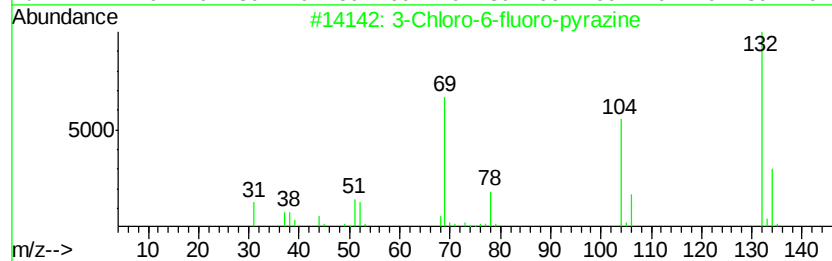
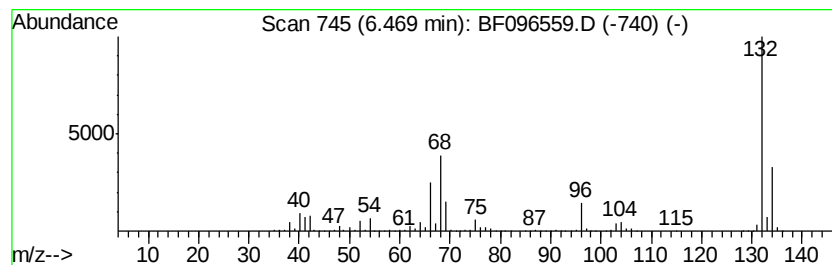
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	80.25 ng	2800840	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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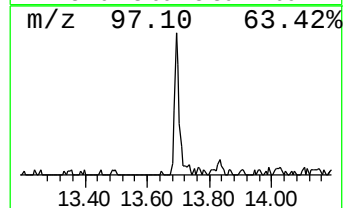
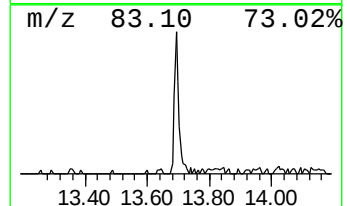
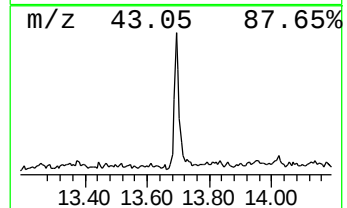
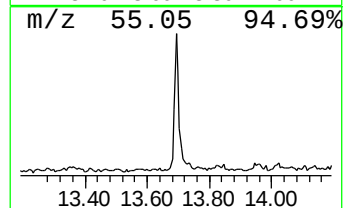
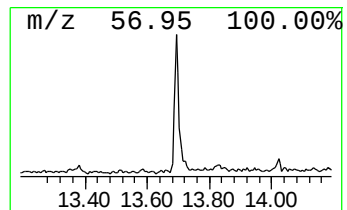
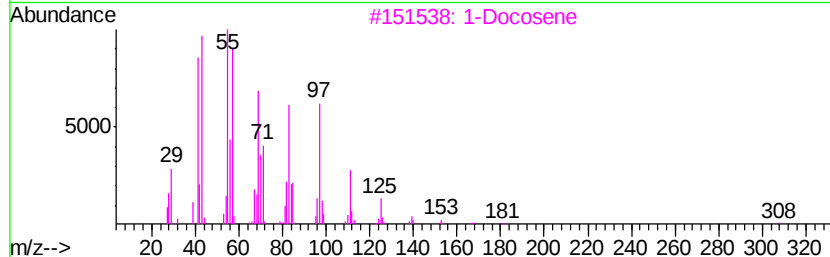
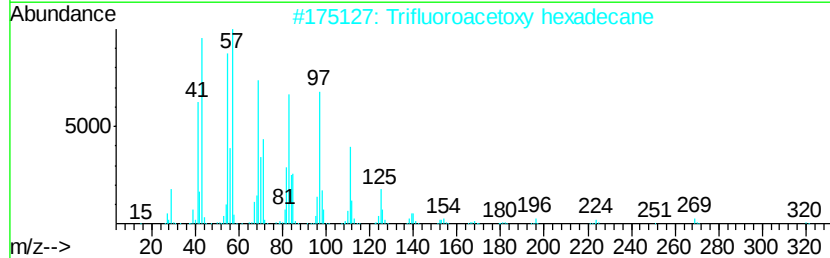
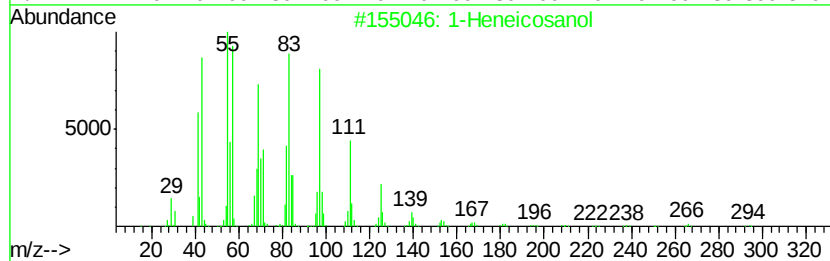
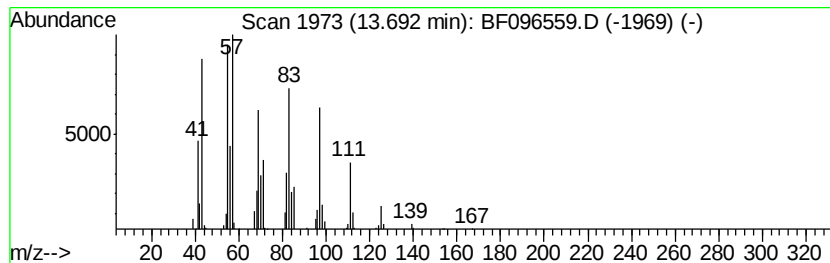
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Peak Number 4 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.69	5.05 ng	164354	Chrysene-d12	13.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	1-Docosene	308	C22H44	001599-67-3	91
4	1-Octadecanol	270	C18H38O	000112-92-5	91
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	91



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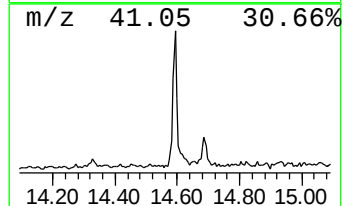
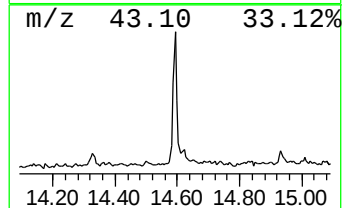
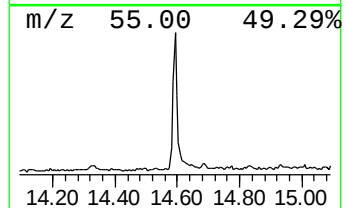
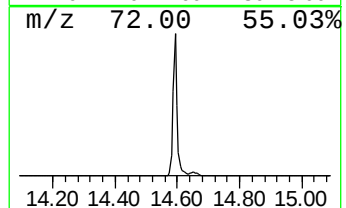
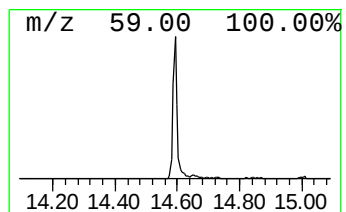
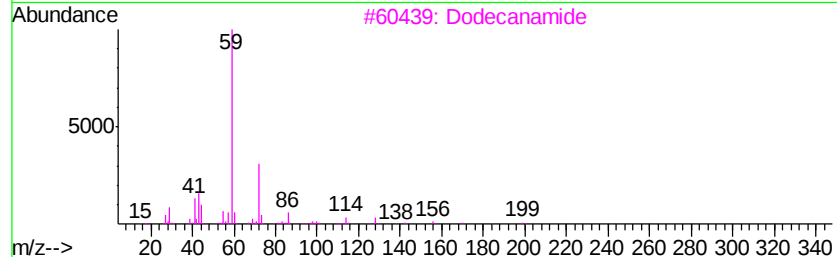
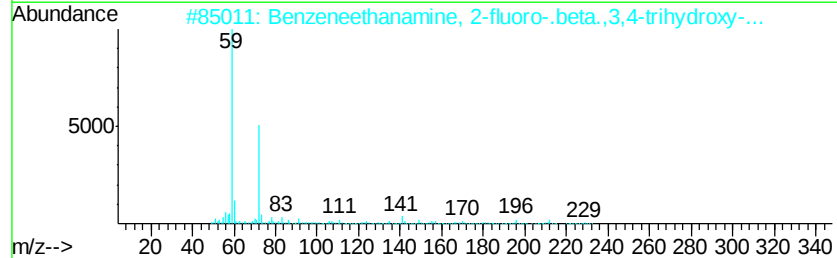
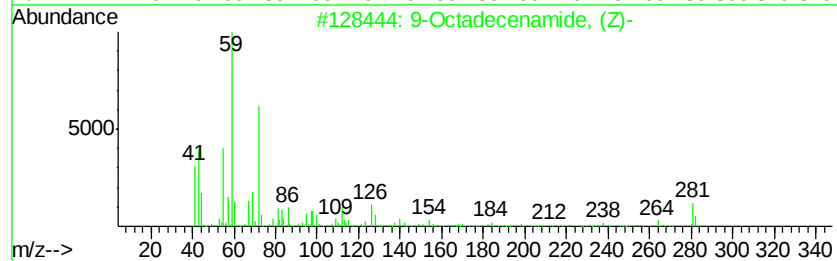
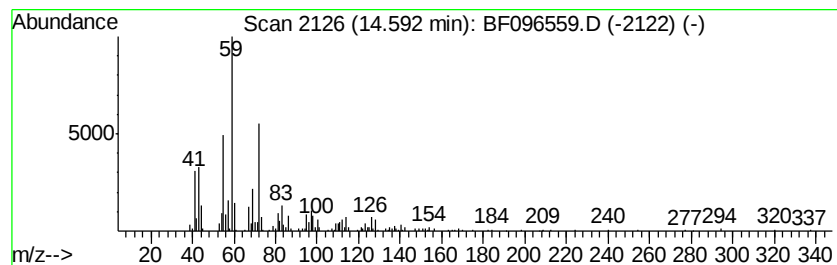
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	12.89 ng	330522	Perylene-d12	15.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0 93
2	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5 64
3	Dodecanamide	199	C12H25NO	001120-16-7 53
4	Phosphonofluoridothioic hydrazid...	156	C3H10FN2PS	036267-52-4 43
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9 43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	17.8	ng	621237	1	6.69	698062	20.0
unknown6.47	6.47	80.3	ng	2800840	1	6.69	698062	20.0
1-Heneicosanol	13.69	5.0	ng	164354	5	13.83	650437	20.0
9-Octadecenamide,...	14.59	12.9	ng	330522	6	15.23	512753	20.0