

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096557.D
 Acq On : 7 Jul 2017 14:20
 Operator : SJ/MA
 Sample : I4064-05
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF002-01

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	4.892	472	477	487	rVB	486171	704360	21.15%	2.456%
2	5.316	543	549	552	rBV	3124057	3252281	97.67%	11.340%
3	6.339	717	723	726	rBV	2994718	3329815	100.00%	11.610%
4	6.469	740	745	748	rBV	3148030	3147173	94.51%	10.974%
5	6.692	780	783	787	rBV	793781	724416	21.76%	2.526%
6	6.851	806	810	814	rBV	2363611	2353213	70.67%	8.205%
7	7.257	873	879	882	rBV	2036371	2083718	62.58%	7.266%
8	7.975	997	1001	1005	rBV	1058508	998976	30.00%	3.483%
9	9.057	1179	1185	1188	rBV	3318202	3283041	98.60%	11.447%
10	9.445	1247	1251	1254	rBV	340942	267047	8.02%	0.931%
11	9.727	1294	1299	1303	rBV2	1106512	989545	29.72%	3.450%
12	10.174	1372	1375	1378	rVB	67854	54187	1.63%	0.189%
13	10.392	1407	1412	1415	rBV3	22859	36215	1.09%	0.126%
14	10.516	1428	1433	1436	rBV	1895459	1879606	56.45%	6.554%
15	10.645	1452	1455	1464	rBV	86809	87066	2.61%	0.304%
16	11.204	1546	1550	1554	rBV	1091847	1014797	30.48%	3.538%
17	12.798	1815	1821	1824	rBV	2430884	2680680	80.51%	9.347%
18	13.692	1969	1973	1982	rBV	212210	236770	7.11%	0.826%
19	13.833	1993	1997	2001	rBV	852401	751408	22.57%	2.620%
20	14.592	2122	2126	2137	rBV	187486	210404	6.32%	0.734%
21	14.686	2139	2142	2146	rBV	49476	50640	1.52%	0.177%
22	15.233	2230	2235	2240	rBV	463970	544223	16.34%	1.898%

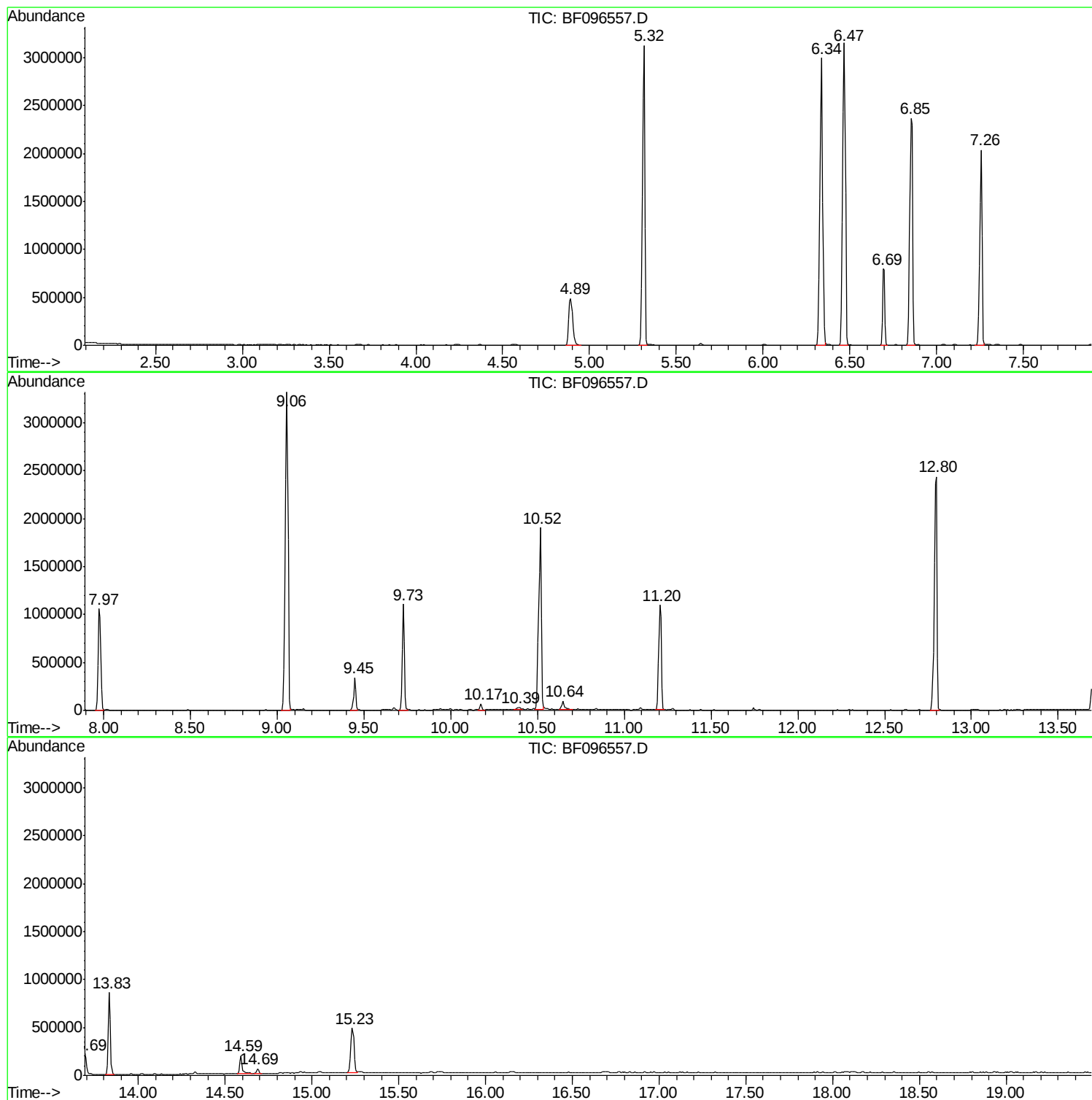
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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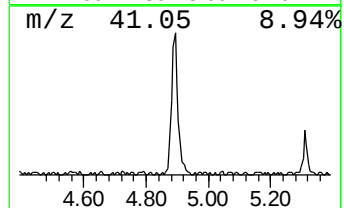
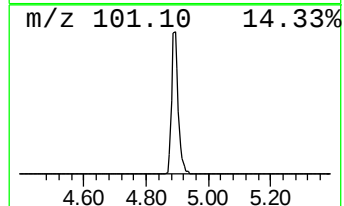
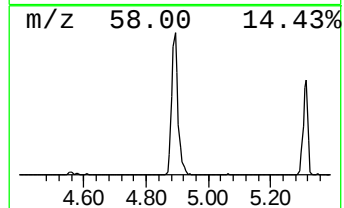
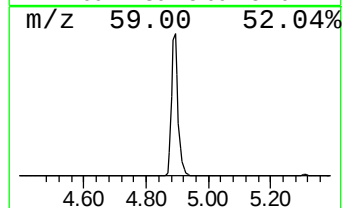
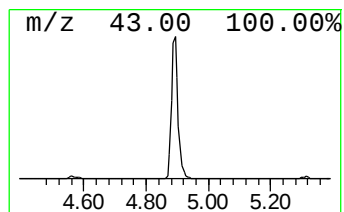
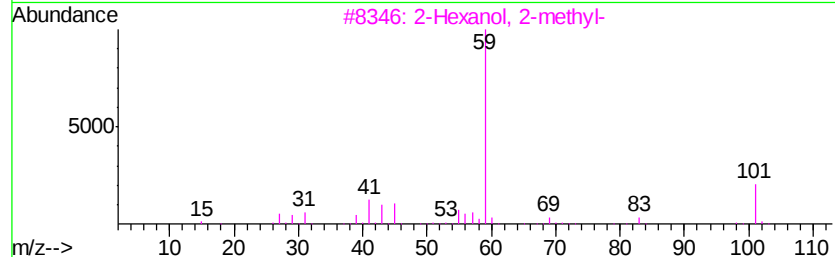
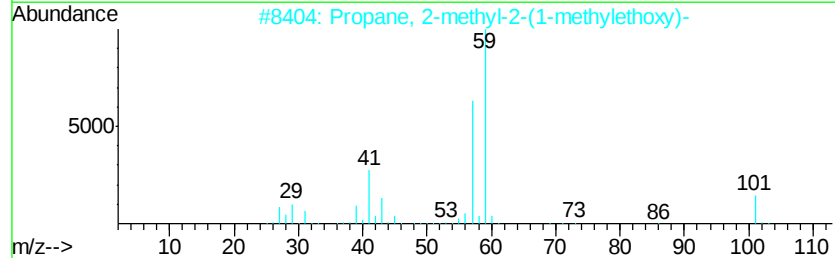
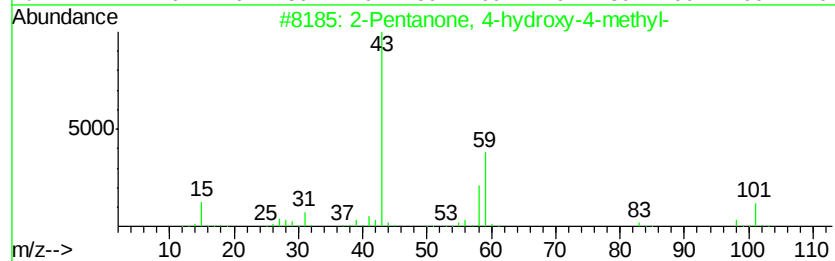
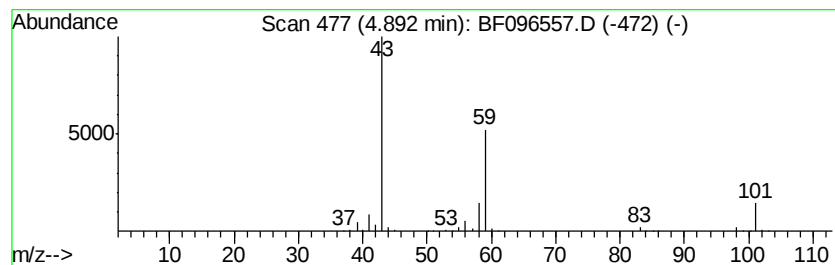
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	19.45 ng	704360	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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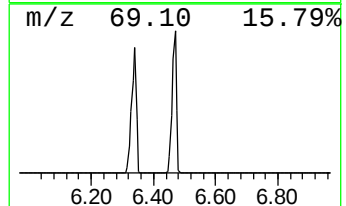
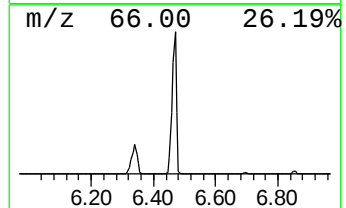
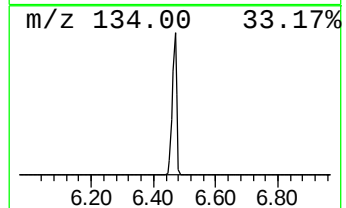
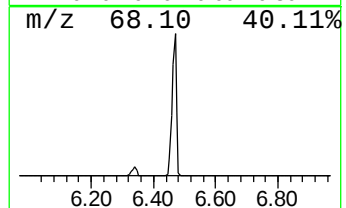
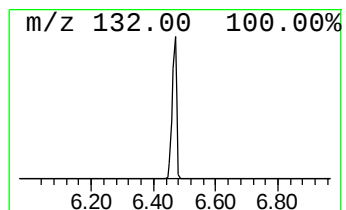
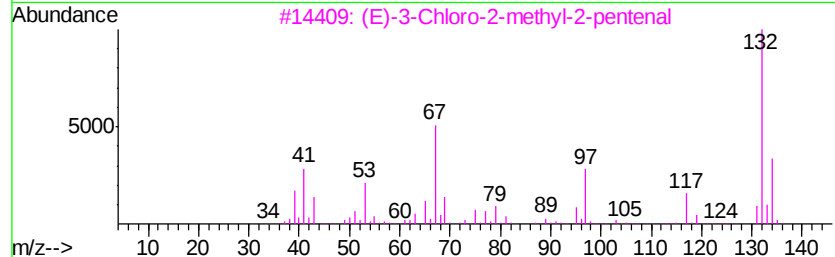
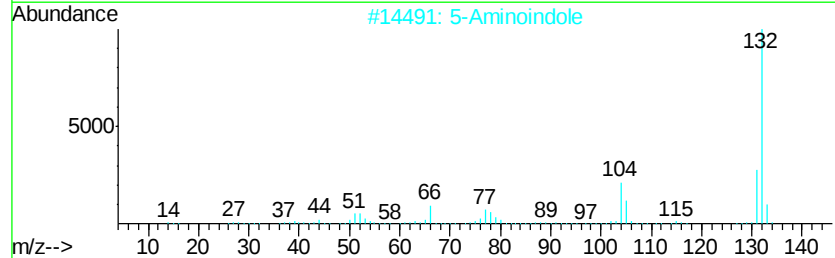
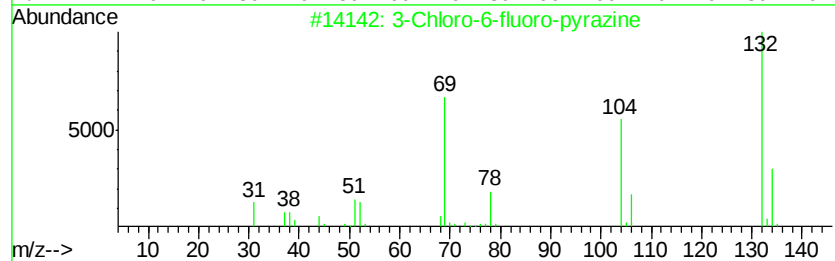
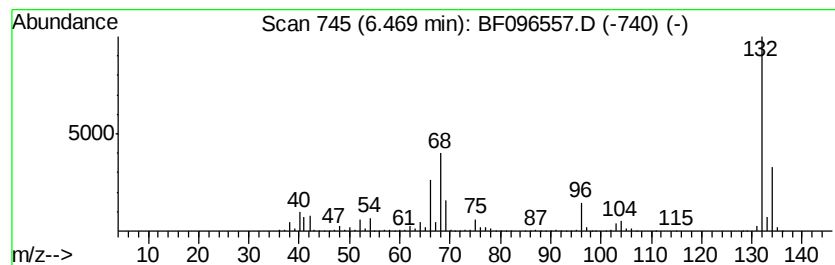
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	86.89 ng	3147170	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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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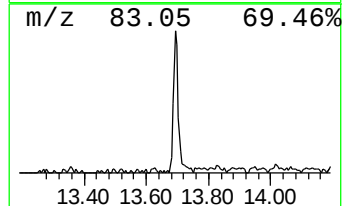
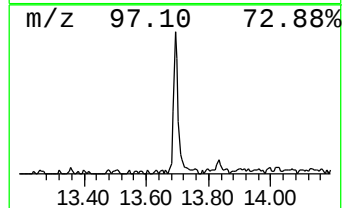
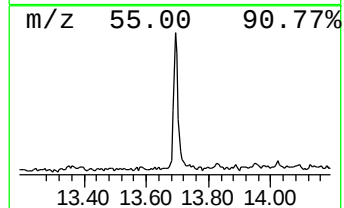
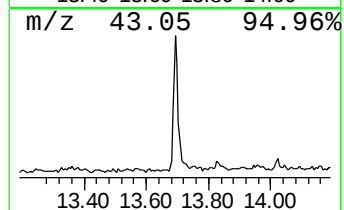
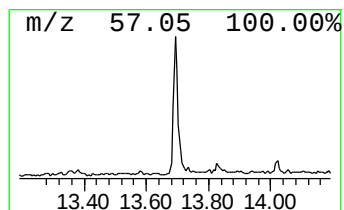
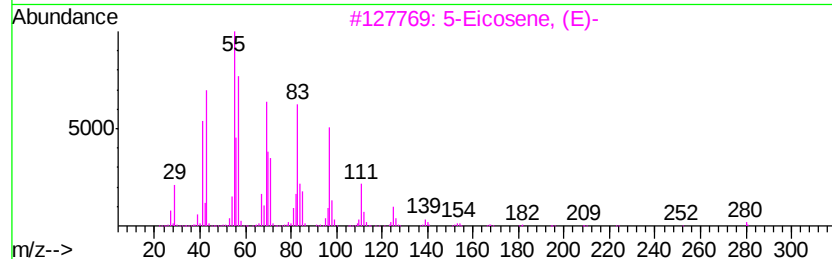
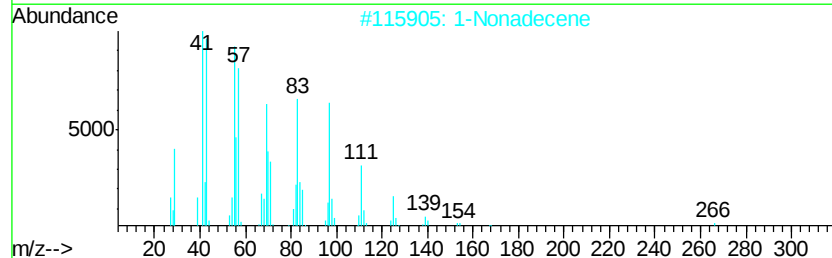
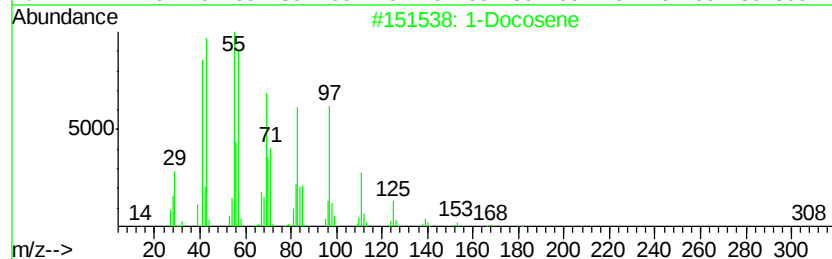
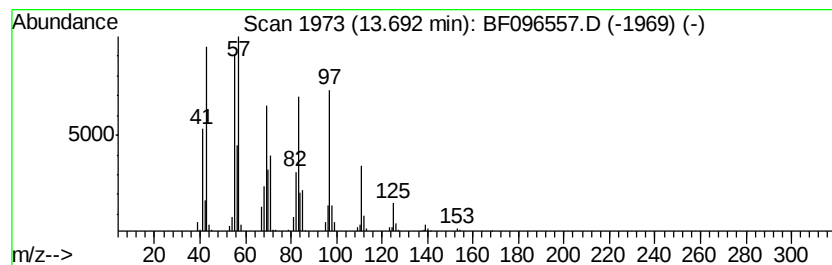
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Peak Number 4 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	6.30 ng	236770	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene		308	C22H44	001599-67-3	95
2	1-Nonadecene		266	C19H38	018435-45-5	91
3	5-Eicosene, (E)-		280	C20H40	074685-30-6	91
4	1-Heneicosanol		312	C21H44O	015594-90-8	91
5	3-Eicosene, (E)-		280	C20H40	074685-33-9	91



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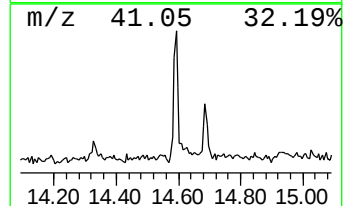
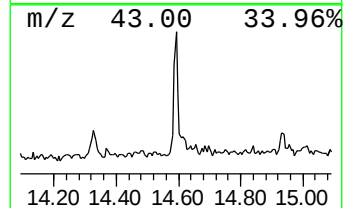
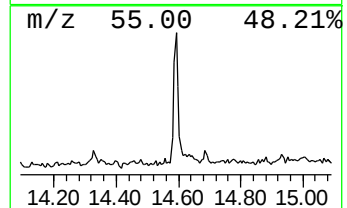
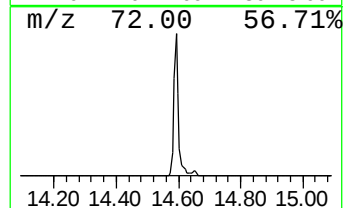
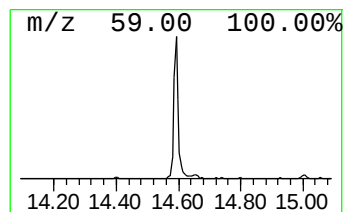
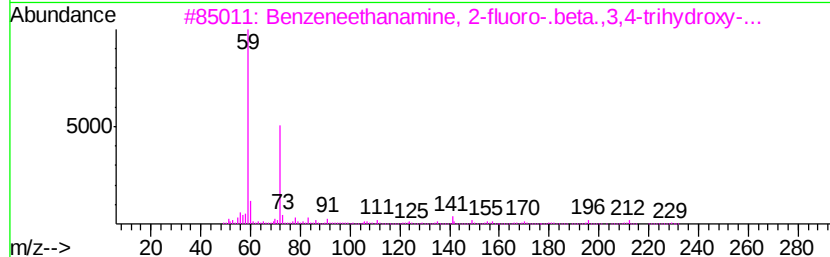
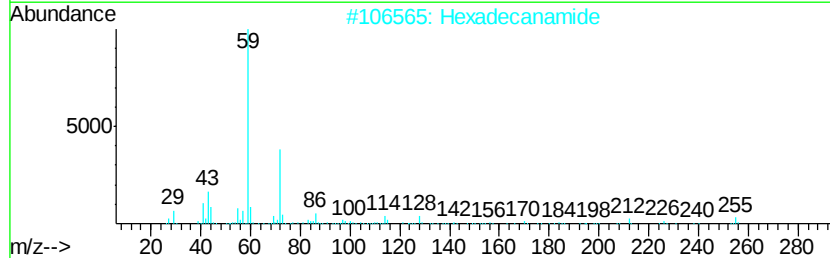
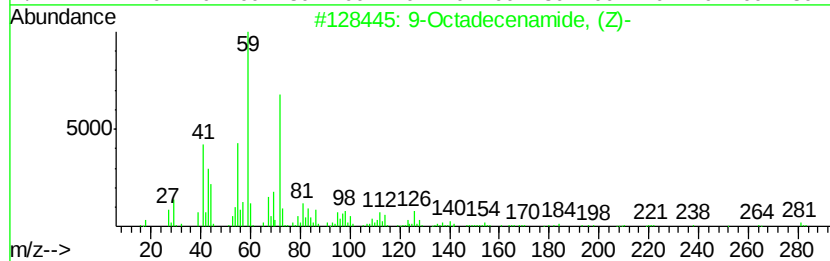
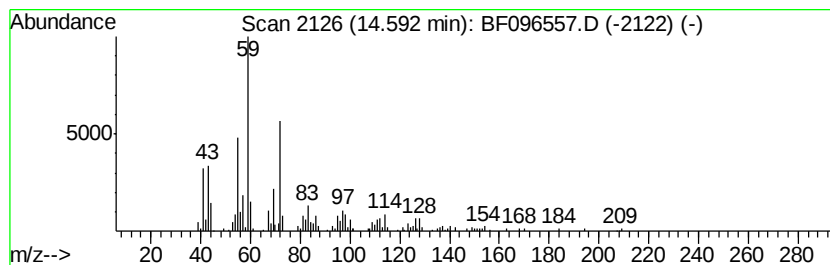
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	7.73 ng	210404	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Decanamide-	171	C10H21NO	002319-29-1	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	19.4	ng	704360	1	6.70	724416	20.0
unknown6.47	6.47	86.9	ng	3147170	1	6.70	724416	20.0
1-Docosene	13.69	6.3	ng	236770	5	13.83	751408	20.0
9-Octadecenamide,...	14.59	7.7	ng	210404	6	15.23	544223	20.0