

Data Path : Z:\HPCHEM1\BNA_F\Data\BF070717\
 Data File : BF096556.D
 Acq On : 7 Jul 2017 13:53
 Operator : SJ/MA
 Sample : I4064-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PET-BF001-02

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	485	rVB	468943	616612	20.53%	2.336%
2	5.310	543	548	552	rBV	2690494	2931580	97.60%	11.105%
3	6.339	717	723	727	rBV	2800667	3003812	100.00%	11.379%
4	6.469	740	745	748	rBV	2910432	2871128	95.58%	10.876%
5	6.698	780	784	787	rBV	805729	718439	23.92%	2.721%
6	6.851	806	810	814	rBV	2154083	2095059	69.75%	7.936%
7	7.257	874	879	882	rBV	1944815	1876155	62.46%	7.107%
8	7.975	997	1001	1005	rBV	1047153	1005759	33.48%	3.810%
9	9.057	1179	1185	1188	rBV	2993249	2847129	94.78%	10.785%
10	9.445	1247	1251	1254	rBV	240025	197983	6.59%	0.750%
11	9.727	1294	1299	1303	rBV2	1227552	1064951	35.45%	4.034%
12	10.175	1372	1375	1378	rVB	55443	41841	1.39%	0.158%
13	10.516	1428	1433	1436	rBV	1724105	1699886	56.59%	6.439%
14	10.645	1452	1455	1463	rVB	62263	61349	2.04%	0.232%
15	11.204	1546	1550	1554	rBV	1109085	1013867	33.75%	3.841%
16	11.745	1637	1642	1646	rBV	31912	30783	1.02%	0.117%
17	12.792	1815	1820	1824	rBV	2407339	2501721	83.28%	9.477%
18	13.692	1969	1973	1981	rBV	278337	275832	9.18%	1.045%
19	13.833	1993	1997	2001	rBV	860046	767786	25.56%	2.908%
20	14.592	2122	2126	2130	rBV	200150	192510	6.41%	0.729%
21	14.686	2138	2142	2145	rBV	44111	41391	1.38%	0.157%
22	15.233	2230	2235	2240	rBV	463746	543132	18.08%	2.057%

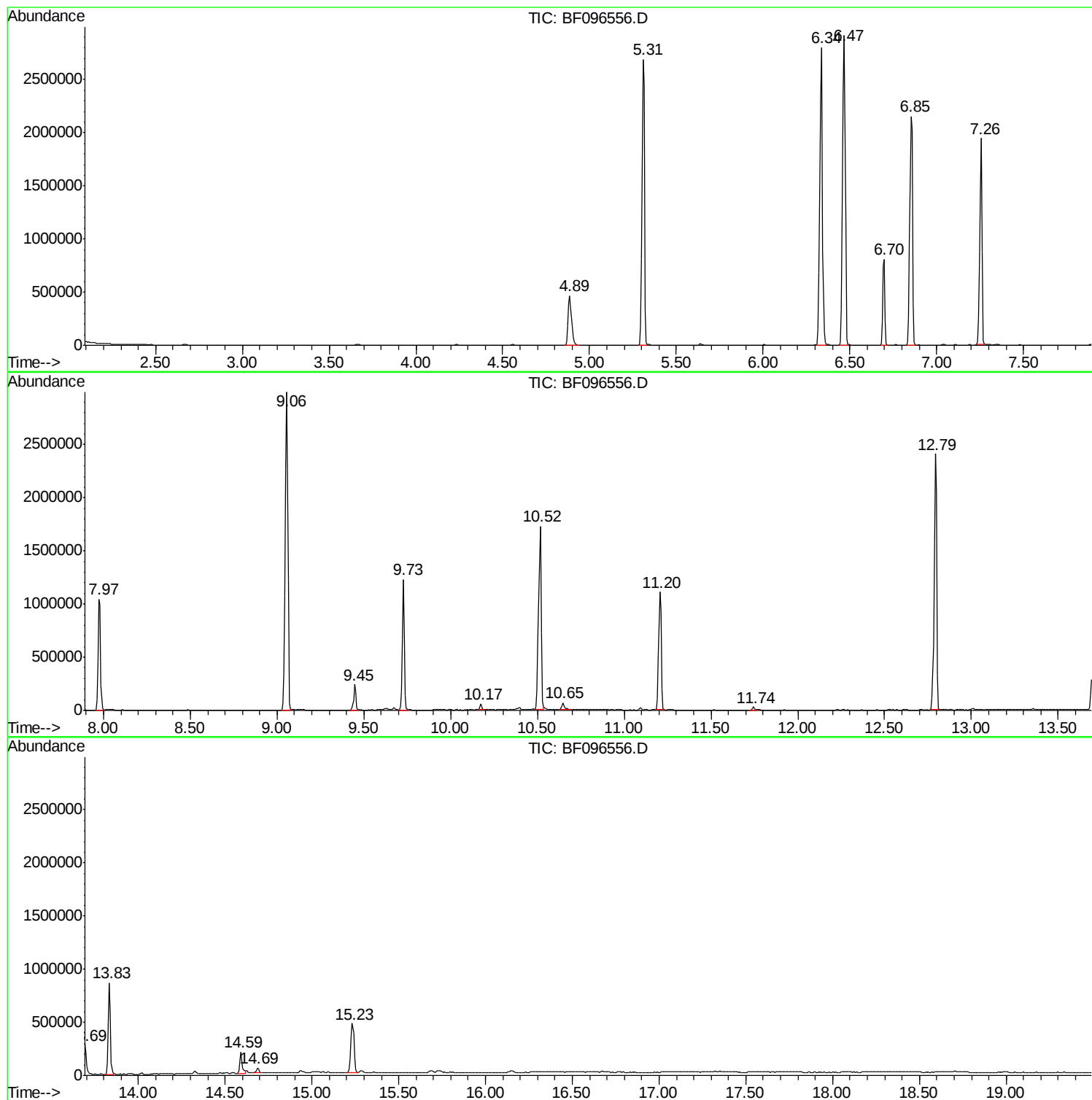
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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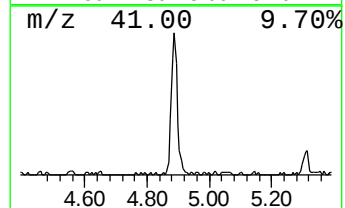
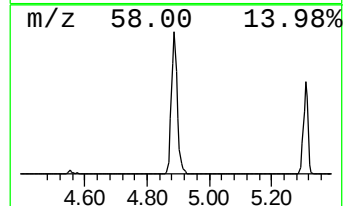
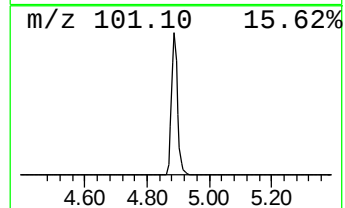
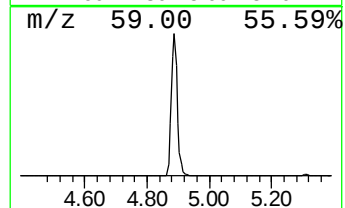
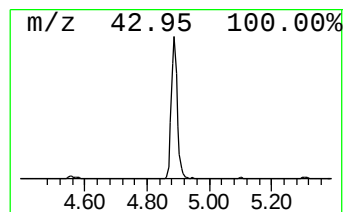
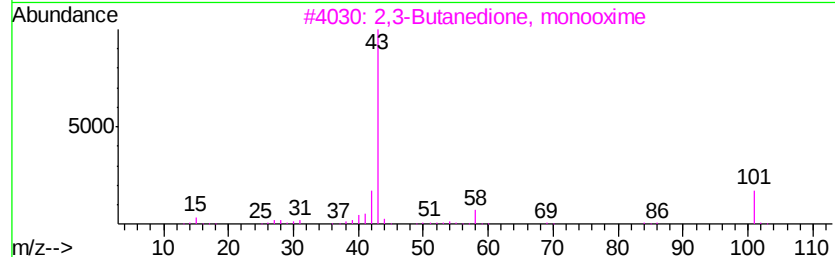
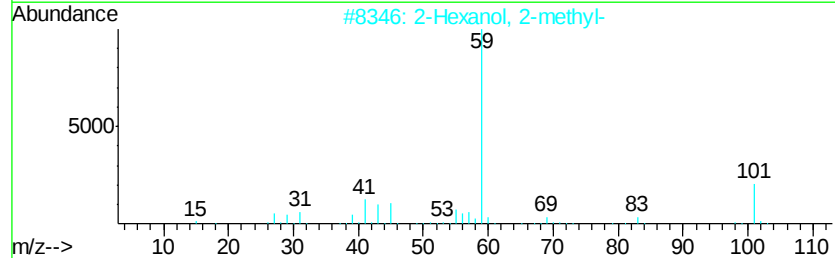
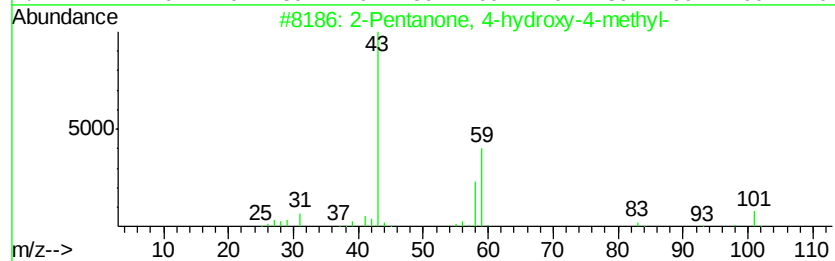
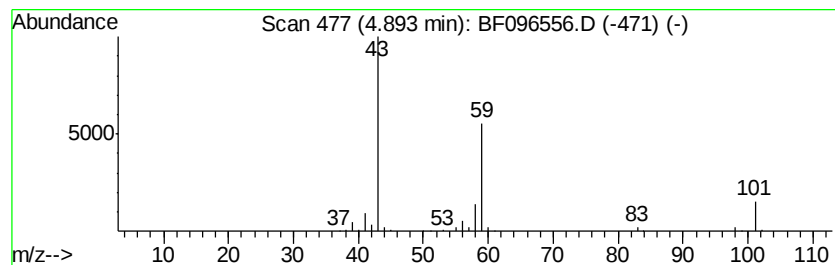
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	17.17 ng	616612	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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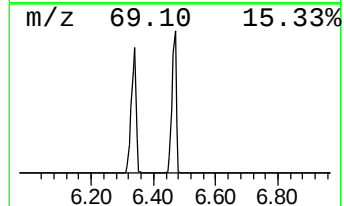
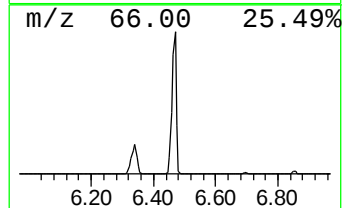
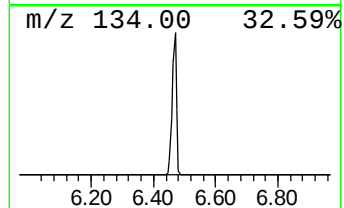
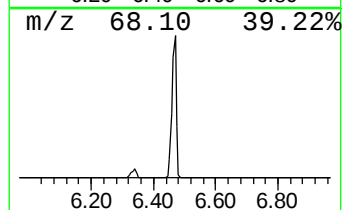
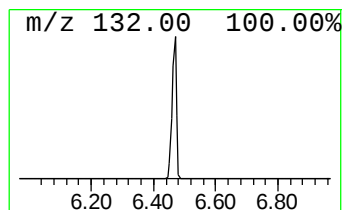
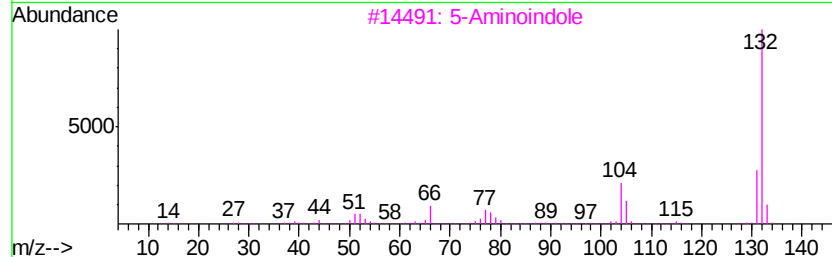
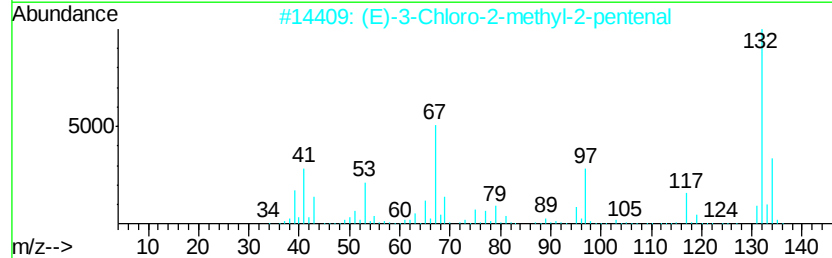
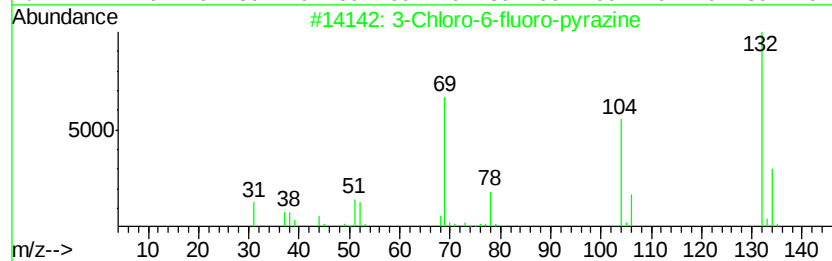
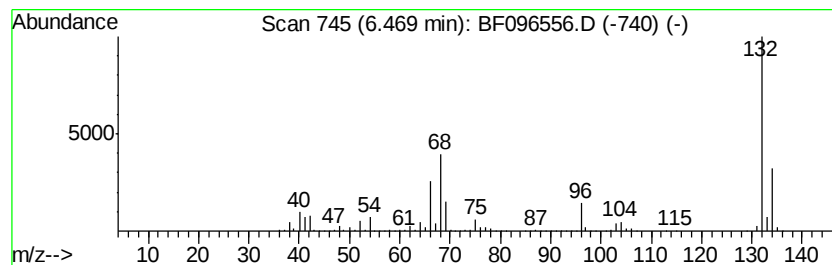
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	79.93 ng	2871130	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		(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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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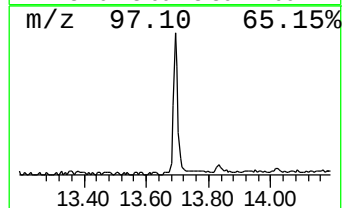
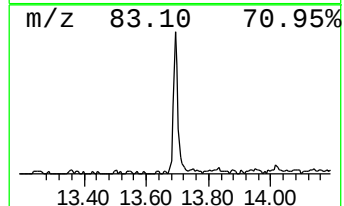
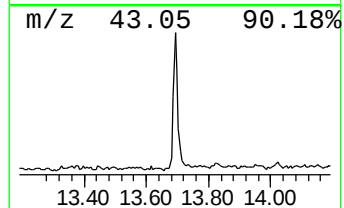
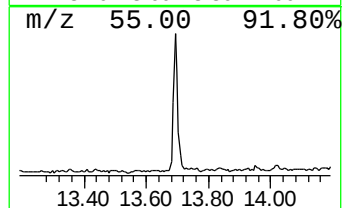
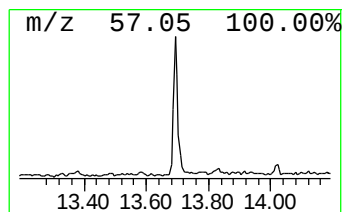
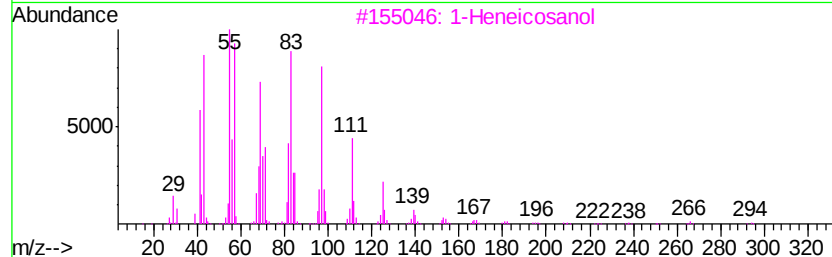
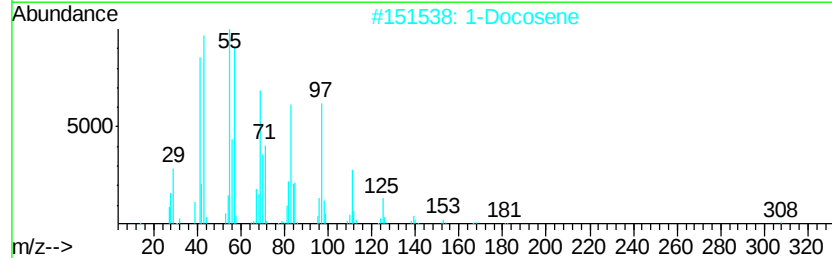
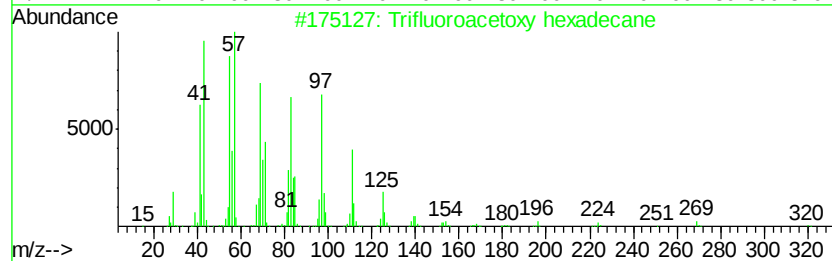
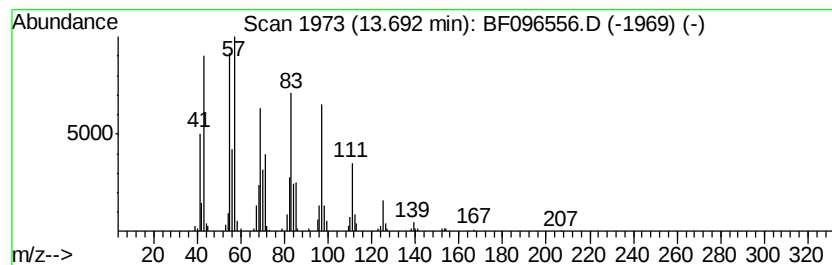
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	7.19 ng	275832	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		1-Docosene	308	C22H44	001599-67-3	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	91
4		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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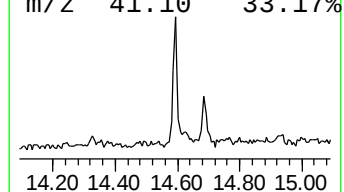
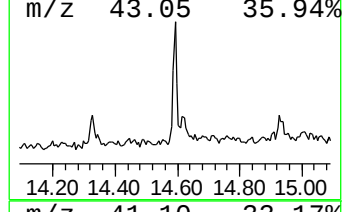
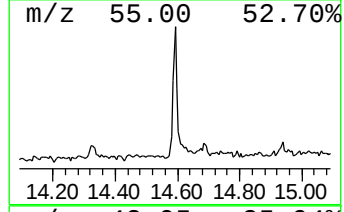
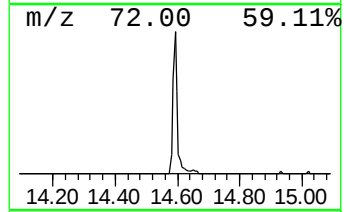
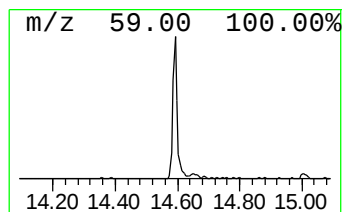
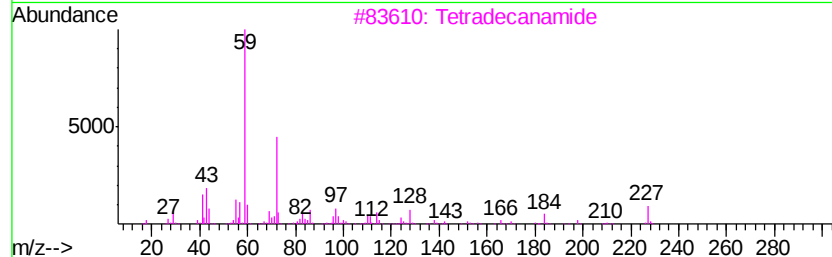
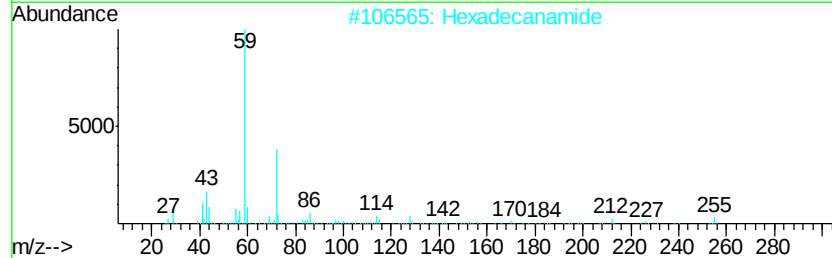
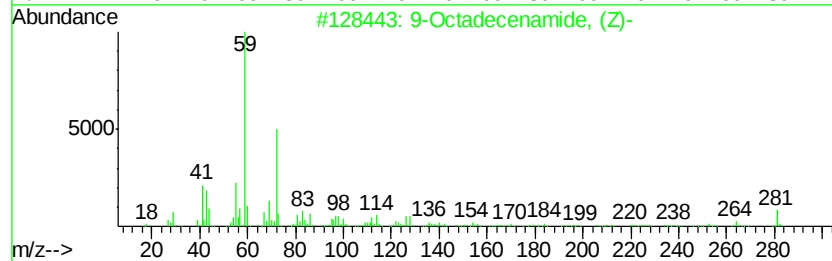
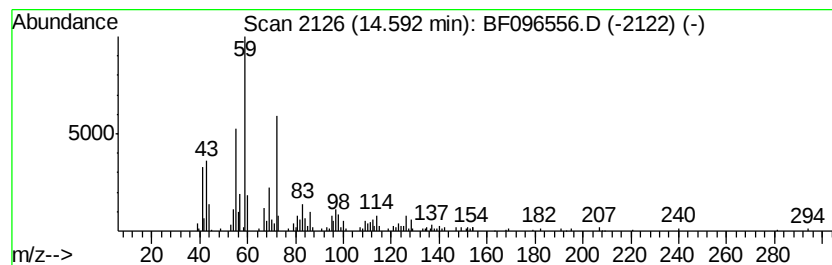
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	7.09 ng	192510	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Hexadecanamide	255	C16H33NO	000629-54-9	78
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		Dodecanamide	199	C12H25NO	001120-16-7	53
5		2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	17.2	ng	616612	1	6.70	718439	20.0
unknown6.47	6.47	79.9	ng	2871130	1	6.70	718439	20.0
Trifluoroacetoxy ...	13.69	7.2	ng	275832	5	13.83	767786	20.0
9-Octadecenamide,...	14.59	7.1	ng	192510	6	15.23	543132	20.0