

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070517\
 Data File : BF096515.D
 Acq On : 6 Jul 2017 6:33
 Operator : SJ/MA
 Sample : I3975-07
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B7-12-14

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:\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	4.910	475	480	492	rBV	294321	457703	15.03%	1.953%
2	5.328	546	551	555	rBV	2694408	3044749	100.00%	12.990%
3	6.357	720	726	729	rBV	2751997	3001192	98.57%	12.804%
4	6.486	743	748	751	rBV	2978435	2878282	94.53%	12.280%
5	6.710	783	786	790	rBV	685636	622615	20.45%	2.656%
6	6.869	809	813	817	rBV	2203942	2149717	70.60%	9.172%
7	7.275	876	882	885	rBV	1812896	1721552	56.54%	7.345%
8	7.992	1000	1004	1008	rBV	860160	754003	24.76%	3.217%
9	9.075	1183	1188	1191	rBV	2775571	2412401	79.23%	10.292%
10	9.469	1250	1255	1258	rBV	899805	751062	24.67%	3.204%
11	9.745	1298	1302	1306	rBV2	714328	634734	20.85%	2.708%
12	10.192	1375	1378	1381	rVB	55872	45676	1.50%	0.195%
13	10.533	1432	1436	1445	rBV	1330028	1240301	40.74%	5.292%
14	10.663	1455	1458	1465	rVB	51212	59263	1.95%	0.253%
15	11.227	1550	1554	1558	rBV	653740	546609	17.95%	2.332%
16	12.651	1791	1796	1801	rBV4	24276	34333	1.13%	0.146%
17	12.815	1820	1824	1827	rBV	2032377	1949330	64.02%	8.317%
18	13.721	1974	1978	1984	rBV	128038	134821	4.43%	0.575%
19	13.857	1998	2001	2005	rBV	604663	601248	19.75%	2.565%
20	15.268	2237	2241	2245	rBV	352674	399022	13.11%	1.702%

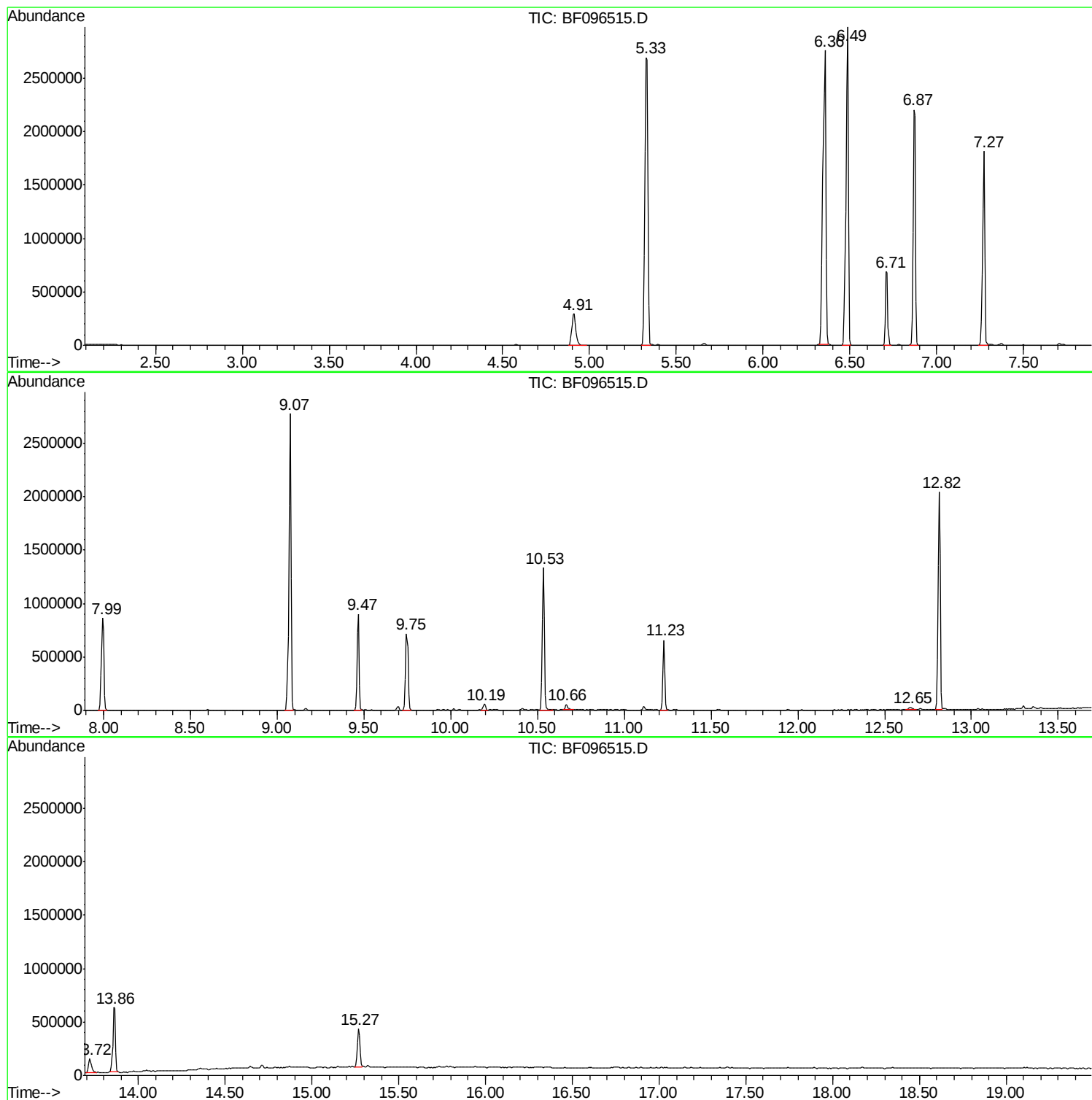
Sum of corrected areas: 23438613

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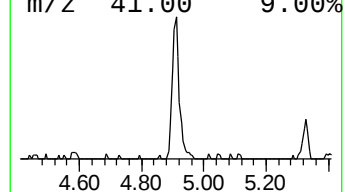
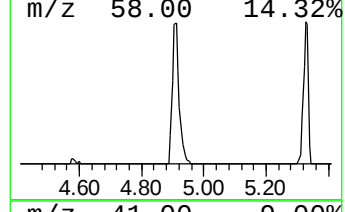
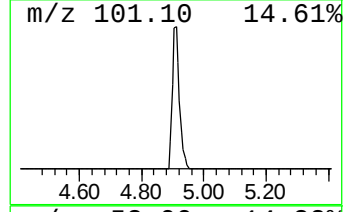
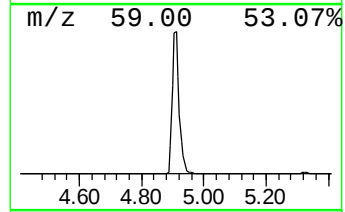
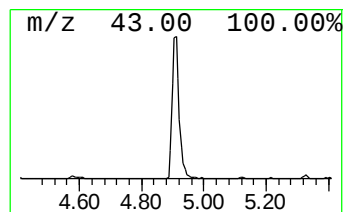
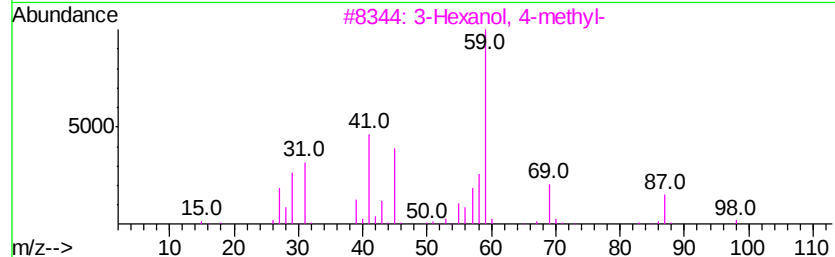
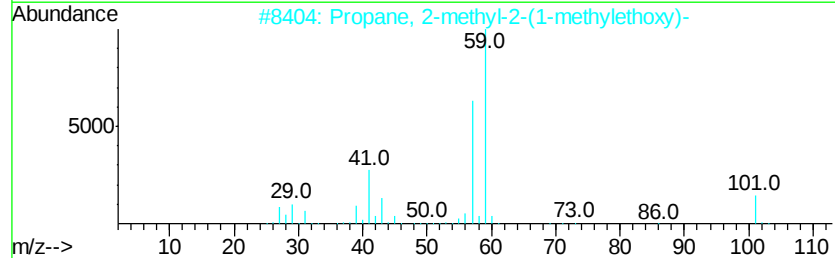
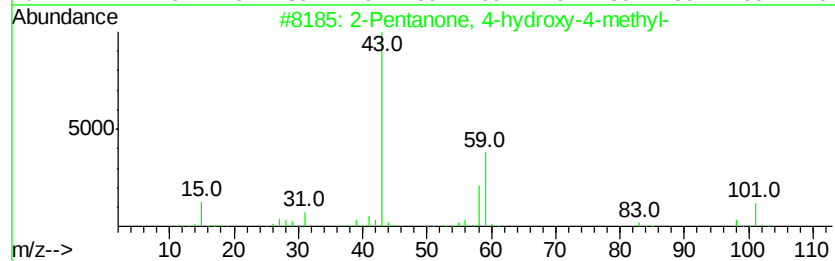
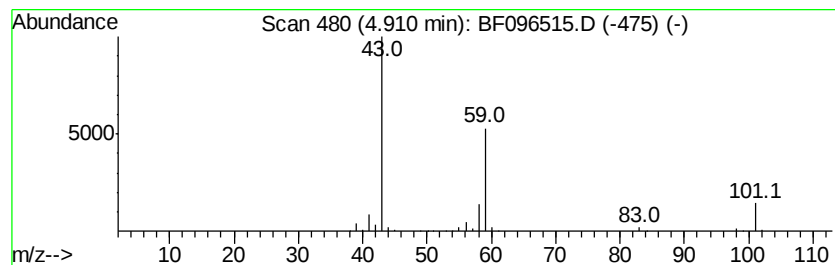
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	14.70 ng	457703	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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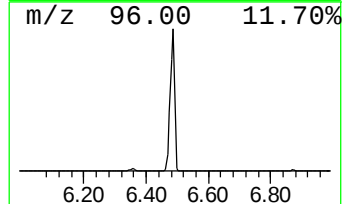
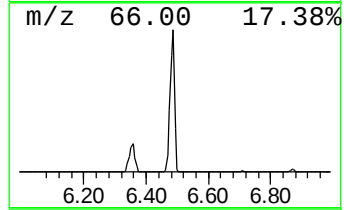
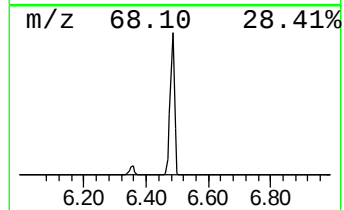
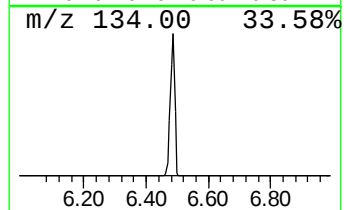
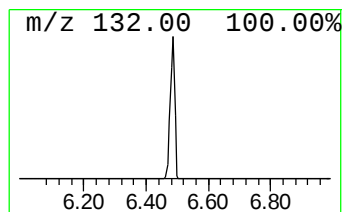
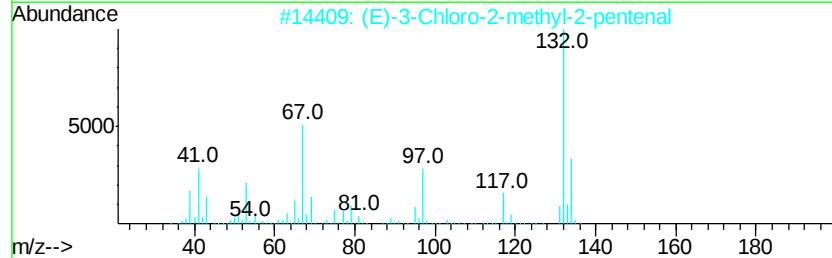
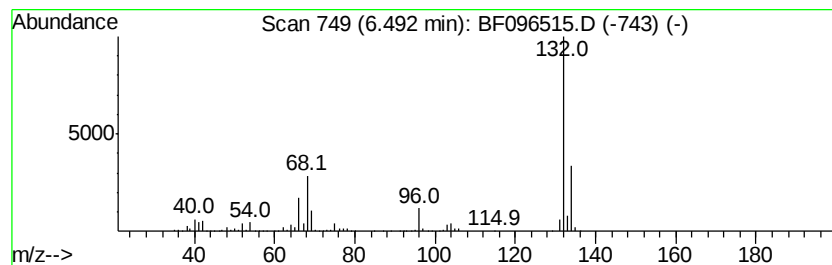
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	92.46 ng	2878280	1,4-Dichlorobenzene-d4	6.72

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	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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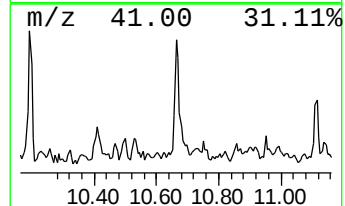
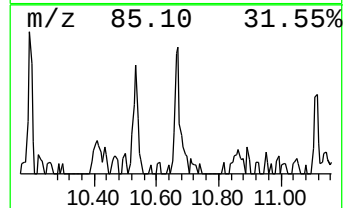
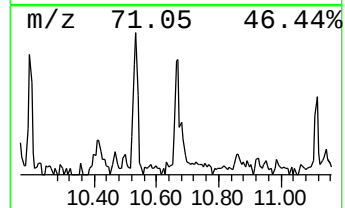
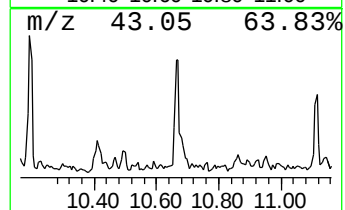
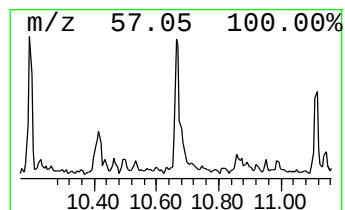
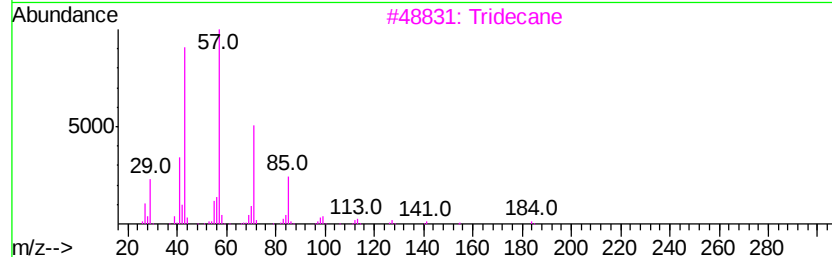
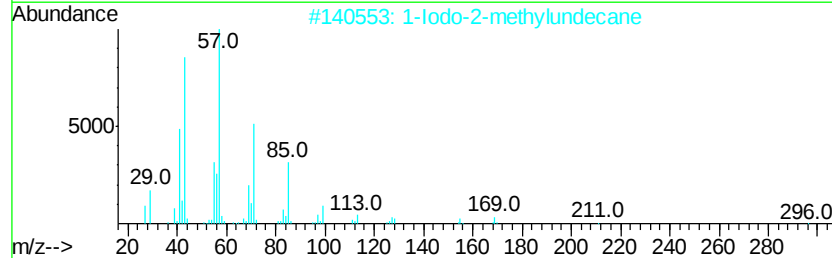
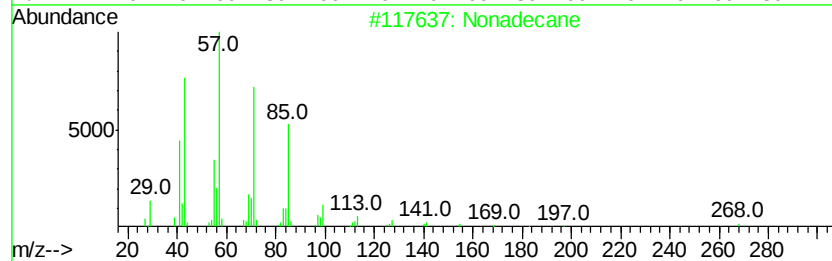
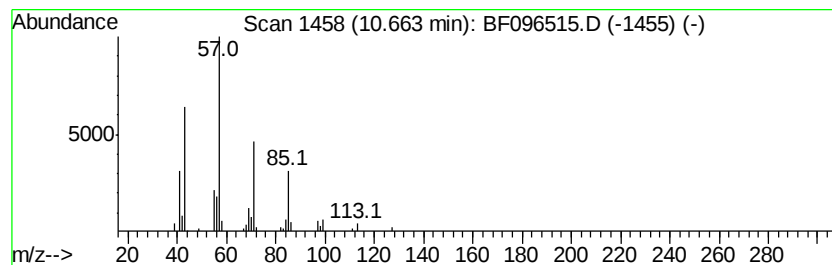
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Peak Number 4 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.66	2.17 ng	59263	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	80
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
3	Tridecane	184	C13H28	000629-50-5	72
4	Pentadecane	212	C15H32	000629-62-9	72
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64



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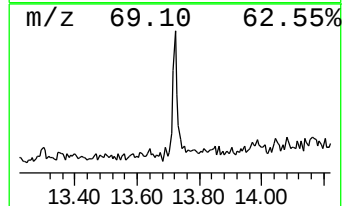
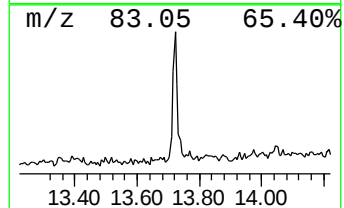
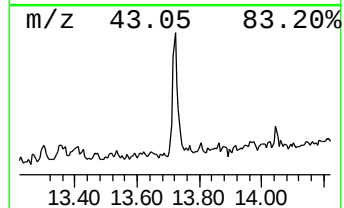
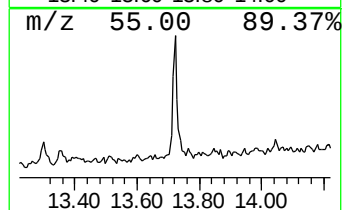
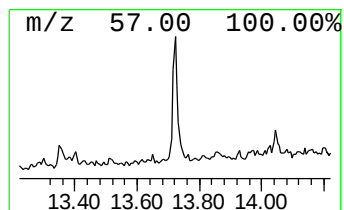
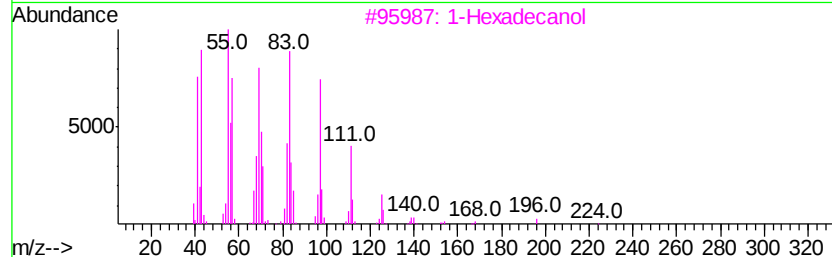
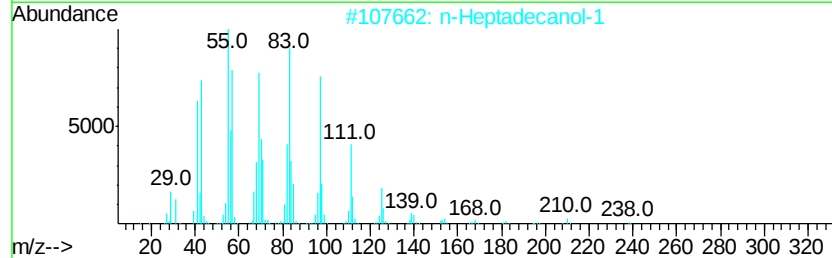
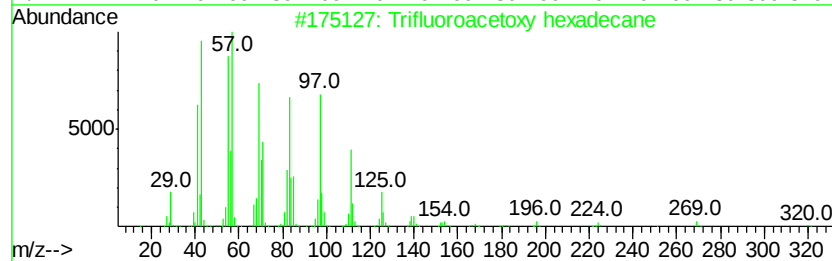
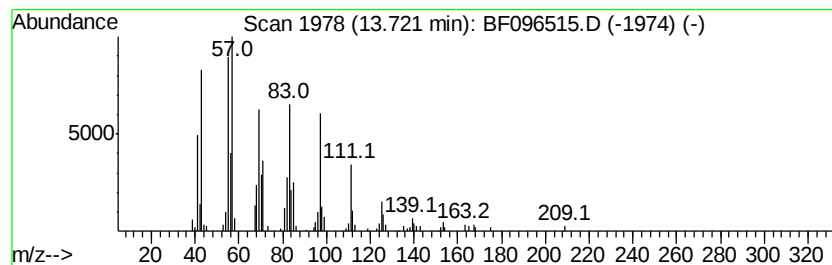
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Peak Number 5 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.48 ng	134821	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3		1-Hexadecanol	242	C16H34O	036653-82-4	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	14.7	ng	457703	1	6.72	622615	20.0
unknown6.49	6.49	92.5	ng	2878280	1	6.72	622615	20.0
Nonadecane	10.66	2.2	ng	59263	4	11.23	546609	20.0
Trifluoroacetoxy ...	13.72	4.5	ng	134821	5	13.86	601248	20.0