

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061917\
 Data File : BF096018.D
 Acq On : 19 Jun 2017 21:40
 Operator : SJ/MA
 Sample : I3745-03
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-GF-02-006-B

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-BF060517.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	1.557	10	12	50	rVB	1437655	2851215	100.00%	16.661%
2	4.492	507	511	529	rBV	63358	191578	6.72%	1.119%
3	5.192	627	630	664	rBV	647751	1479896	51.90%	8.648%
4	6.875	912	916	927	rBV	806709	1345532	47.19%	7.863%
5	6.963	927	931	956	rVB	1036841	1836426	64.41%	10.731%
6	7.304	985	989	1008	rVB	308146	421684	14.79%	2.464%
7	7.539	1024	1029	1048	rBV	921355	1264193	44.34%	7.387%
8	8.222	1141	1145	1169	rBV	546806	914485	32.07%	5.344%
9	9.333	1330	1334	1351	rBV	350281	556551	19.52%	3.252%
10	11.116	1631	1637	1650	rBV	1449951	1809222	63.45%	10.572%
11	11.815	1752	1756	1773	rBV	84729	135681	4.76%	0.793%
12	12.157	1809	1814	1826	rBV2	423152	571205	20.03%	3.338%
13	13.451	2030	2034	2058	rBV	495574	796004	27.92%	4.651%
14	14.551	2217	2221	2237	rVB	322002	485152	17.02%	2.835%
15	15.574	2391	2395	2403	rBV2	41528	53165	1.86%	0.311%
16	16.386	2530	2533	2541	rBV	34245	47168	1.65%	0.276%
17	16.692	2580	2585	2594	rBV2	40624	66661	2.34%	0.390%
18	16.927	2620	2625	2634	rVB2	1041550	1210767	42.46%	7.075%
19	18.186	2835	2839	2848	rBV	55250	88841	3.12%	0.519%
20	18.274	2850	2854	2866	rBV	318945	466269	16.35%	2.725%
21	19.415	3044	3048	3054	rBV3	27024	41969	1.47%	0.245%
22	19.562	3069	3073	3076	rBV	30780	39233	1.38%	0.229%
23	19.844	3118	3121	3126	rBV	21175	32325	1.13%	0.189%
24	19.944	3135	3138	3146	rVV	294384	408024	14.31%	2.384%

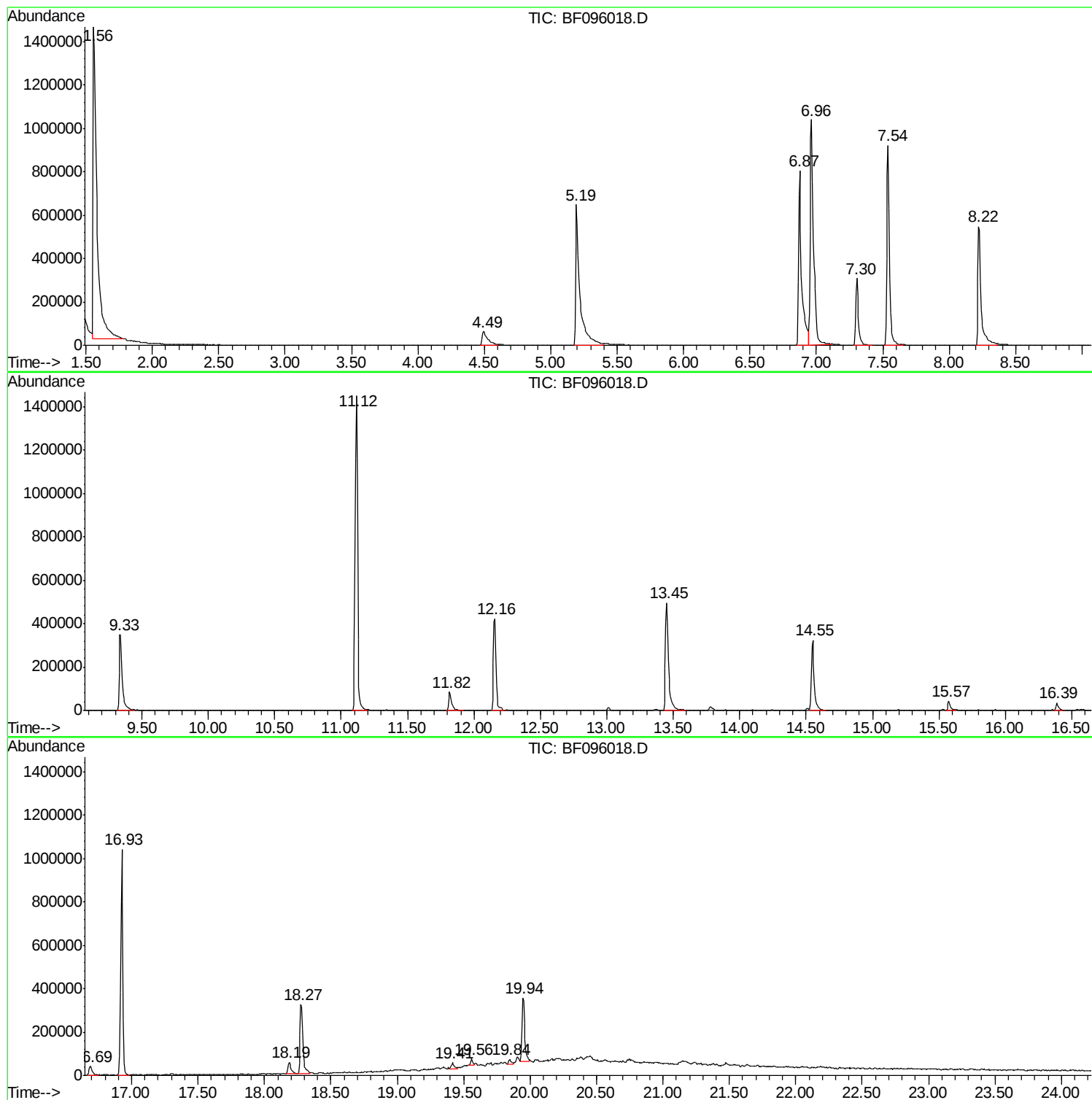
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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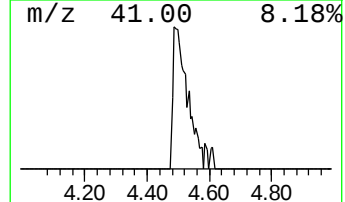
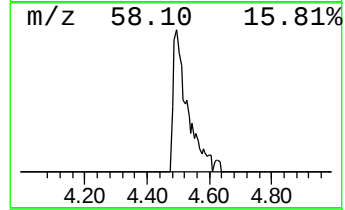
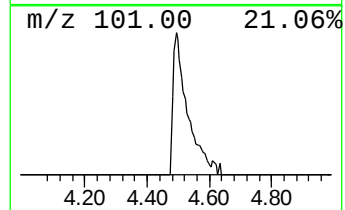
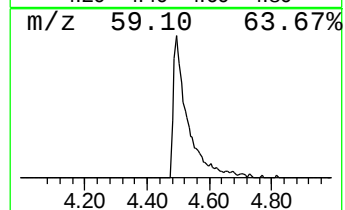
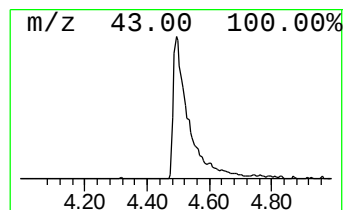
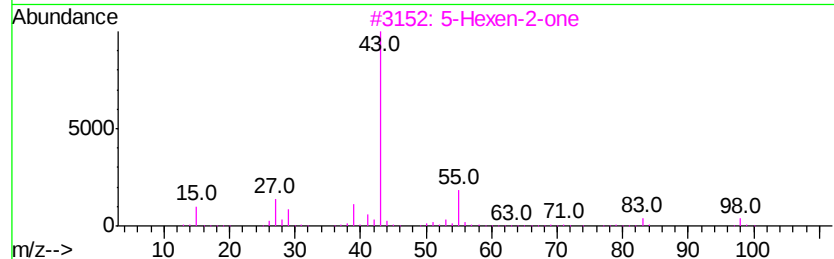
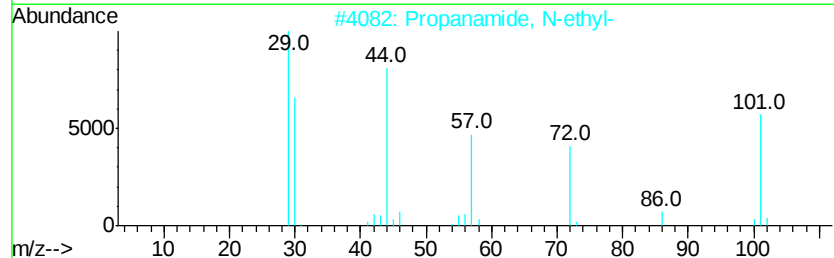
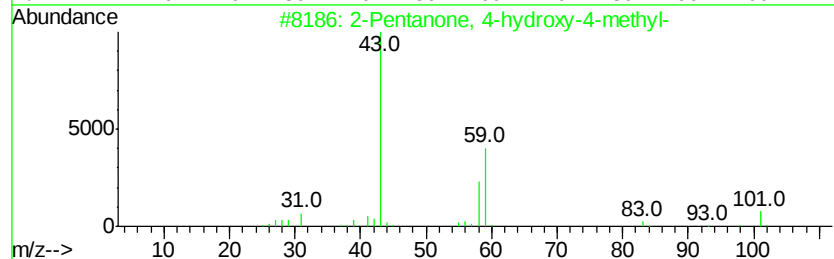
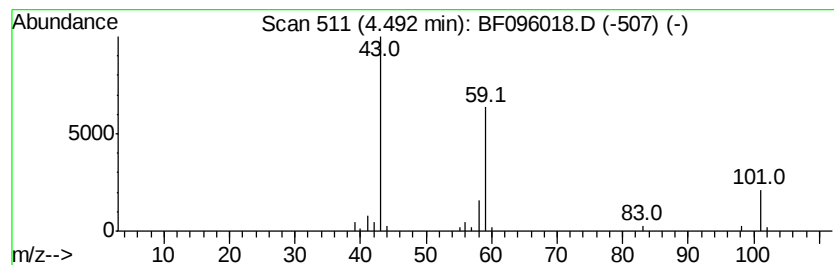
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	9.09 ng	191578	1,4-Dichlorobenzene-d4	7.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Propanamide, N-ethyl-	101	C5H11NO	005129-72-6	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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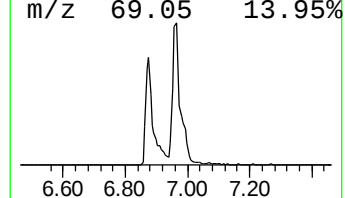
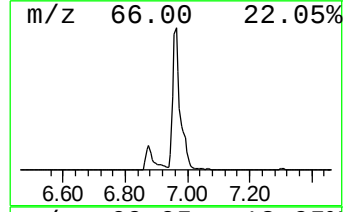
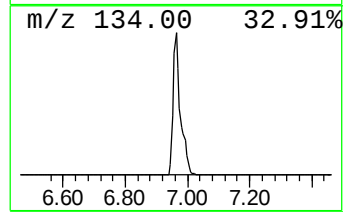
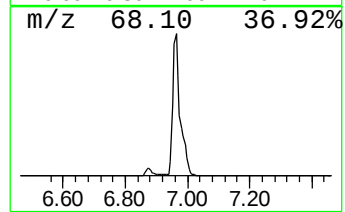
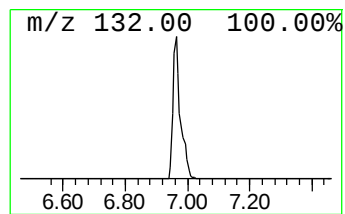
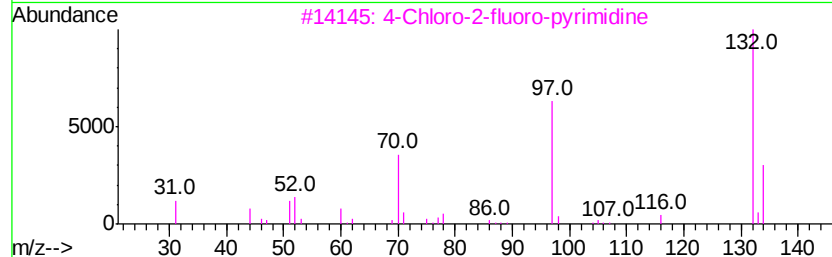
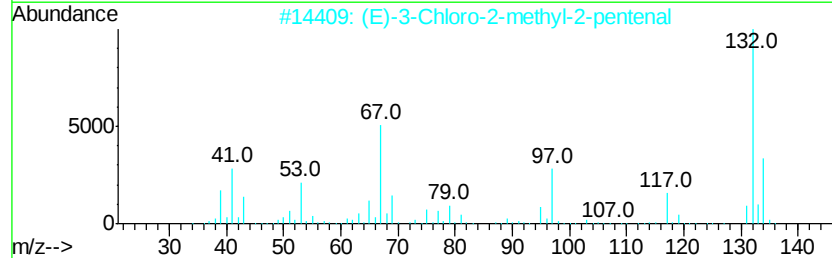
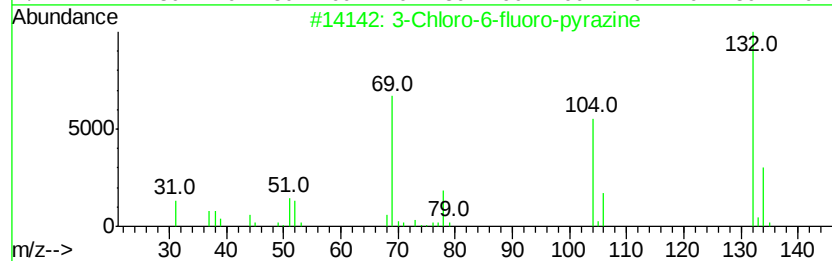
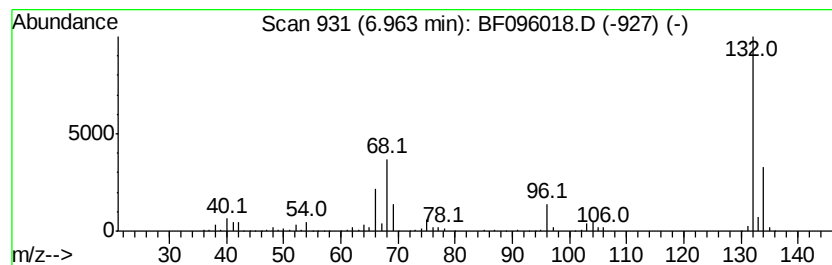
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Peak Number 3 unknown6.96 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	87.10 ng	1836430	1,4-Dichlorobenzene-d4	7.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3		Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	4		Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	5		Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	5		Aminoindole	132	C8H8N2	005192-03-0	9



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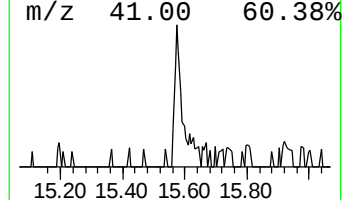
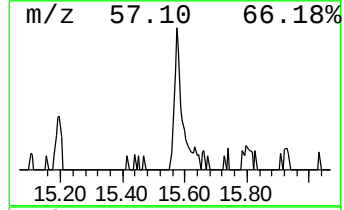
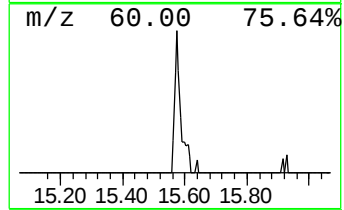
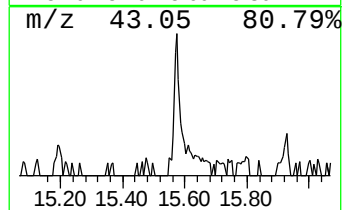
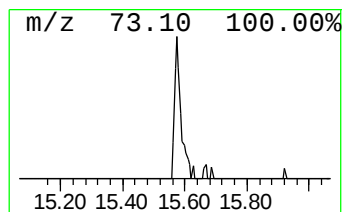
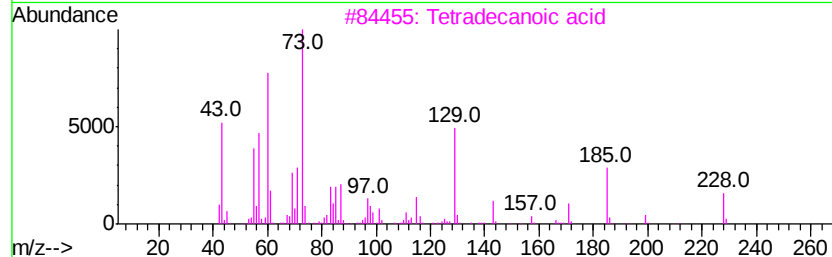
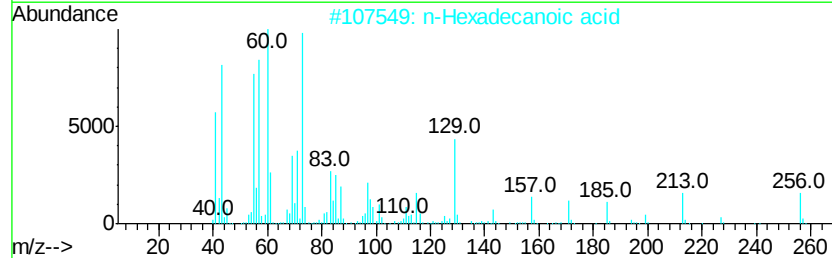
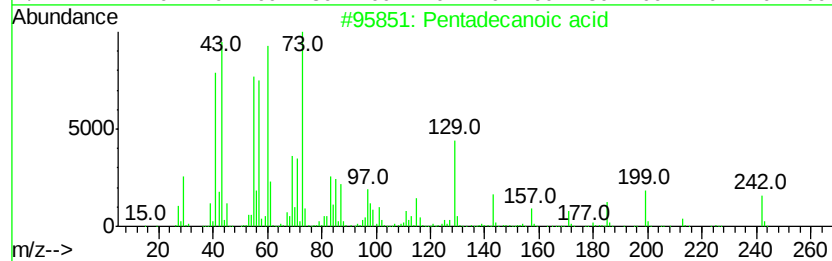
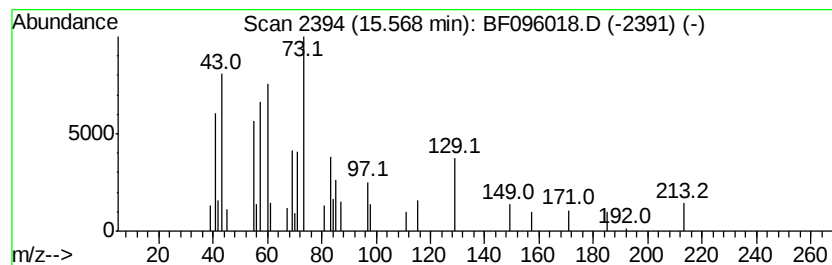
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Peak Number 5 Pentadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	2.19 ng	53165	Phenanthrene-d10	14.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	72
5		Dodecanoic acid	200	C12H24O2	000143-07-7	64



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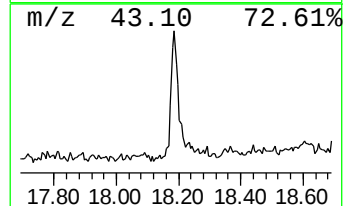
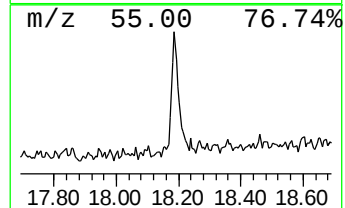
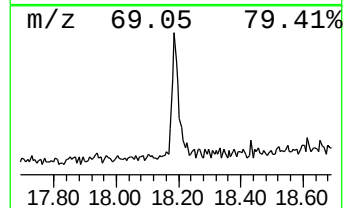
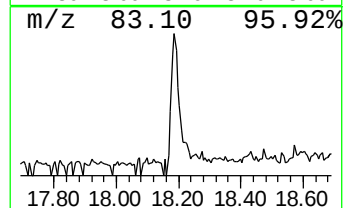
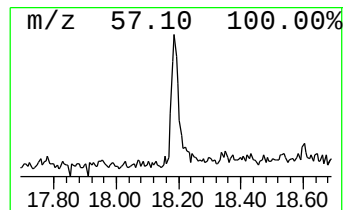
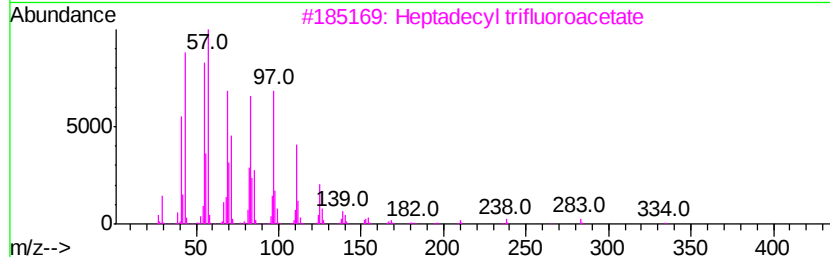
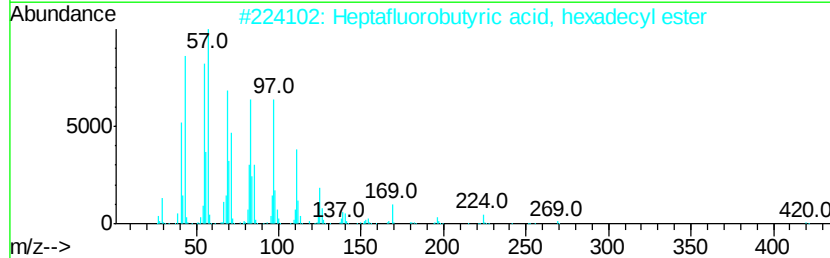
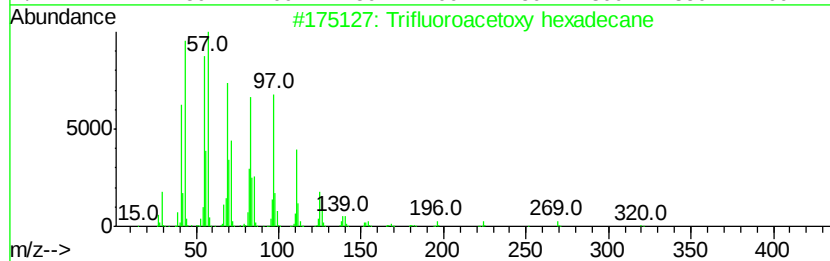
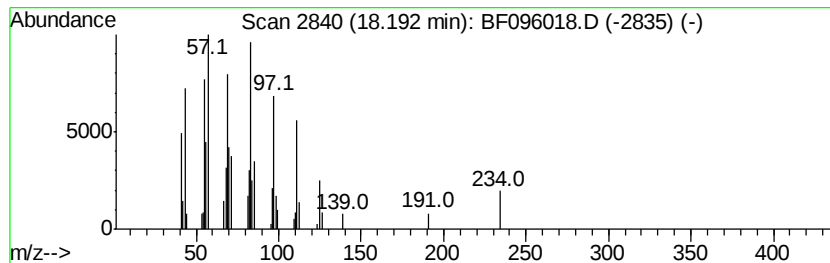
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Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.19	3.81 ng	88841	Chrysene-d12	18.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	93
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
4		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	93
5		Trichloroacetic acid, hexadecyl ester	386	C18H33Cl3O2	074339-54-1	91



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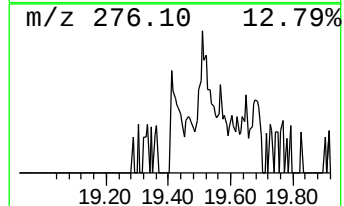
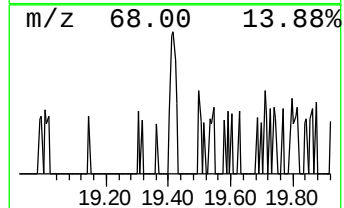
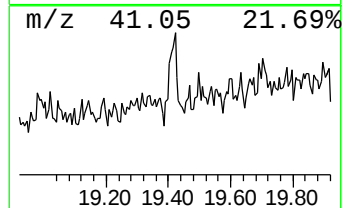
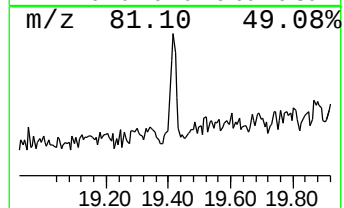
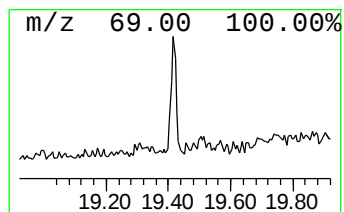
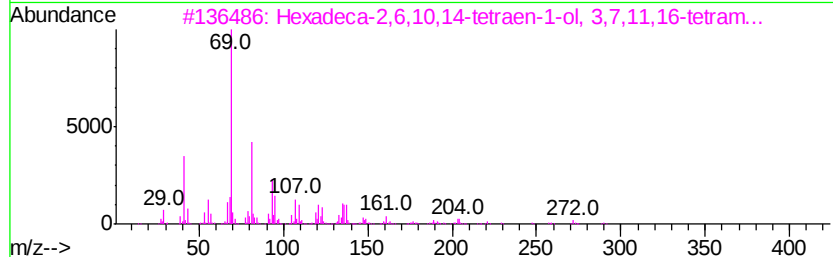
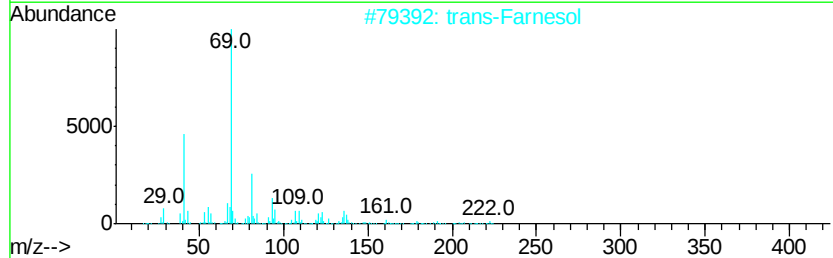
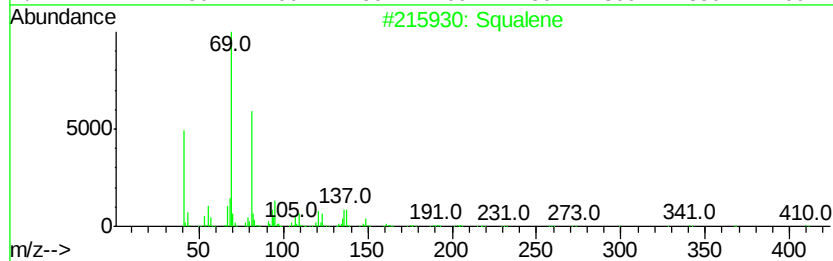
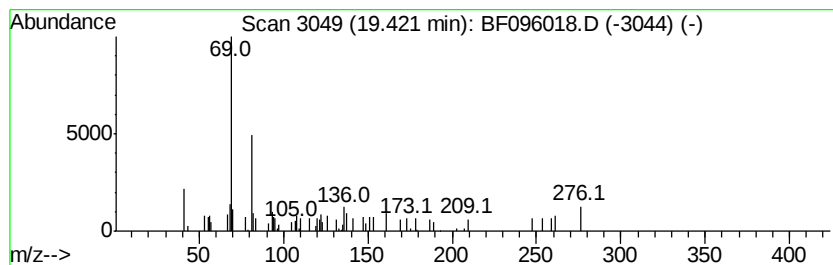
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Peak Number 8 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.42	2.06 ng	41969	Perylene-d12		19.94
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	53
2	trans-Farnesol	222	C15H26O	000106-28-5	53
3	Hexadeca-2,6,10,14-tetraen-1-ol, ...	290	C20H34O	007614-21-3	53
4	Supraene	410	C30H50	007683-64-9	53
5	Nerolidol 1	222	C15H26O	1000285-43-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.49	9.1	ng	191578	1	7.30	421684	20.0
unknown6.96	6.96	87.1	ng	1836430	1	7.30	421684	20.0
Pentadecanoic acid	15.57	2.2	ng	53165	4	14.55	485152	20.0
Trifluoroacetoxy ...	18.19	3.8	ng	88841	5	18.28	466269	20.0
Squalene	19.42	2.1	ng	41969	6	19.94	408024	20.0