

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090716\
 Data File : BF090007.D
 Acq On : 7 Sep 2016 16:17
 Operator : UM/SJ
 Sample : H4676-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RAMP-A(0-2)-6

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-BF083116.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	1.736	11	13	62	rVB	3627190	9538105	100.00%	15.620%
2	4.753	274	277	291	rBV	675773	1360598	14.26%	2.228%
3	5.199	313	316	336	rBV	4068582	5384978	56.46%	8.819%
4	6.262	406	409	412	rBV	3199106	5444108	57.08%	8.915%
5	6.387	417	420	422	rBV	4309617	5481329	57.47%	8.976%
6	6.616	438	440	451	rVB	960857	1127813	11.82%	1.847%
7	6.776	451	454	456	rBV	3071015	4119892	43.19%	6.747%
8	7.187	487	490	492	rBV	3025388	3629631	38.05%	5.944%
9	7.896	550	552	563	rBV	1212070	1483424	15.55%	2.429%
10	8.982	644	647	649	rBV	5673616	5850726	61.34%	9.581%
11	9.382	679	682	684	rBV	538475	788743	8.27%	1.292%
12	9.645	703	705	715	rVB	1852597	1753458	18.38%	2.872%
13	10.102	738	745	746	rBV2	88274	141561	1.48%	0.232%
14	10.434	771	774	776	rBV	3265048	3866470	40.54%	6.332%
15	10.571	784	786	790	rBV	117923	161080	1.69%	0.264%
16	11.119	831	834	836	rBV	1551609	1845550	19.35%	3.022%
17	12.697	969	972	975	rBV	4005961	5849061	61.32%	9.579%
18	13.611	1049	1052	1058	rBV	116883	185868	1.95%	0.304%
19	13.725	1060	1062	1065	rBV	1455947	1460408	15.31%	2.392%
20	15.063	1177	1179	1182	rBV	802910	1115563	11.70%	1.827%
21	16.331	1287	1290	1294	rBV	192566	377348	3.96%	0.618%
22	17.486	1386	1391	1399	rBV4	32317	98433	1.03%	0.161%

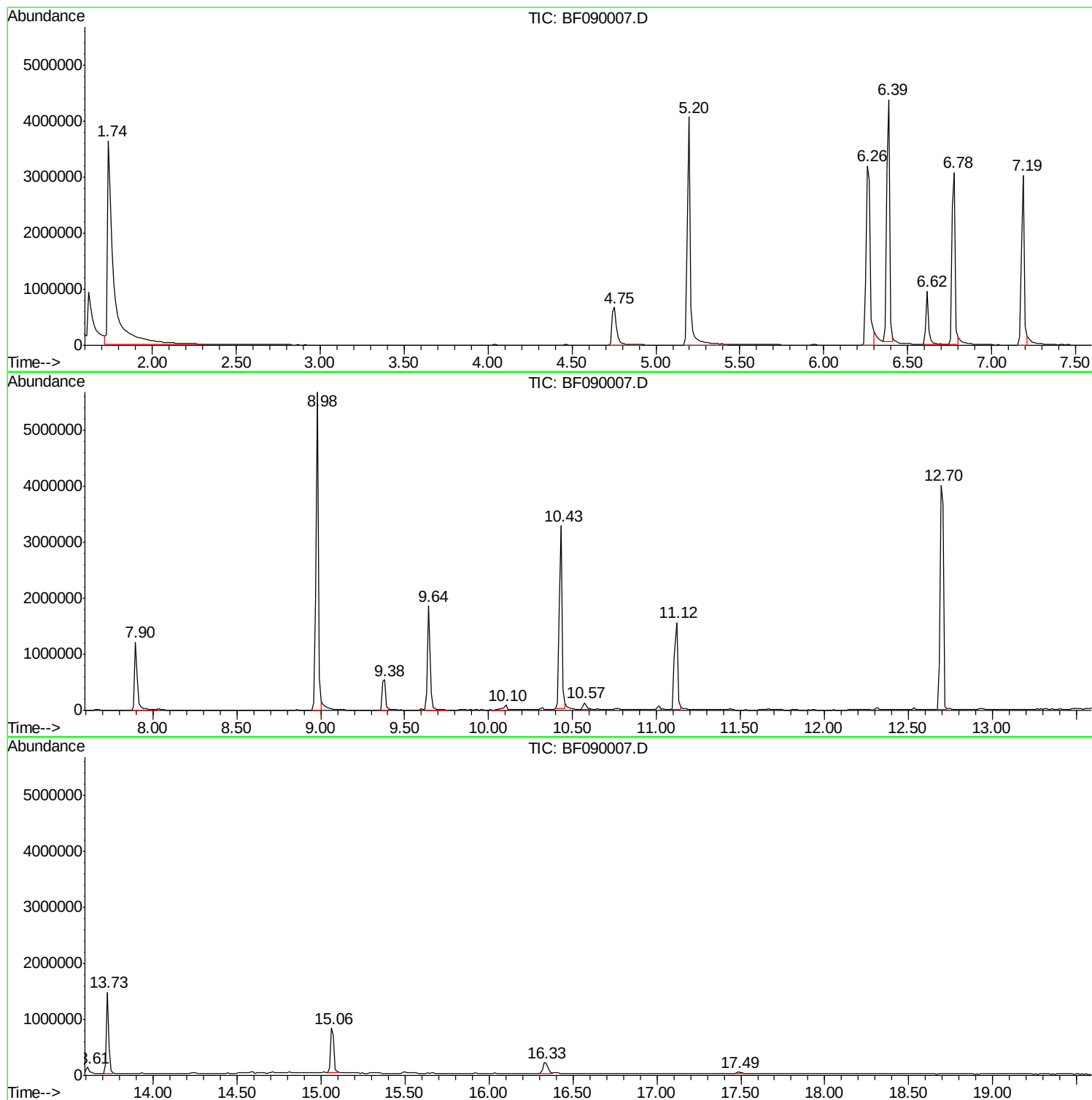
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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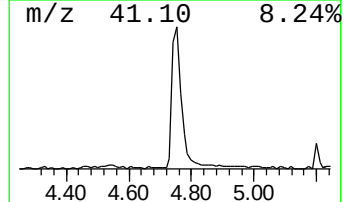
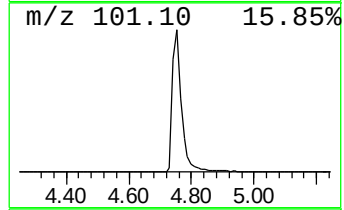
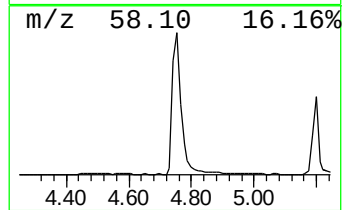
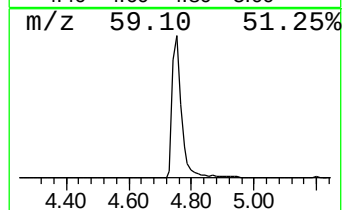
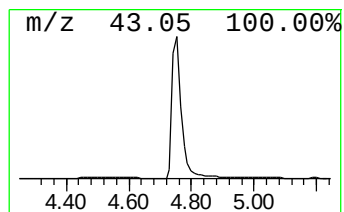
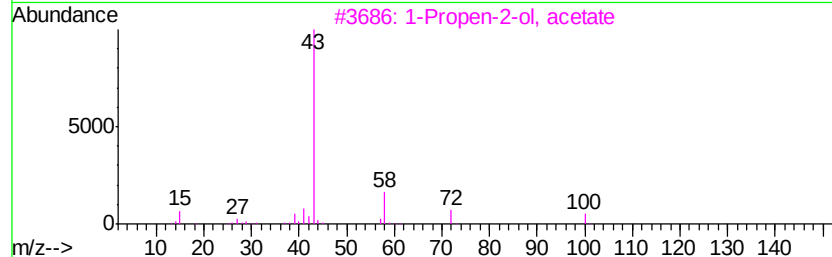
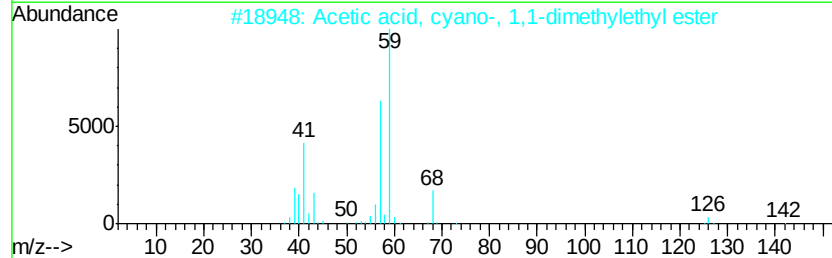
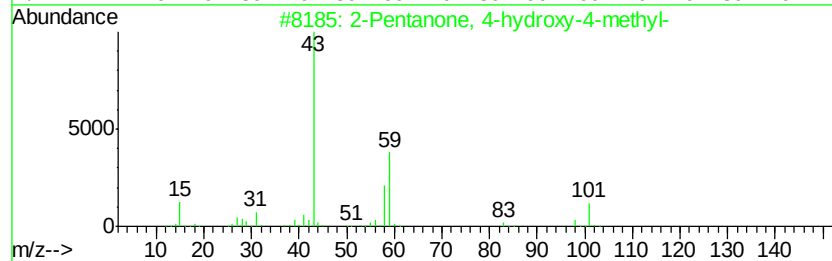
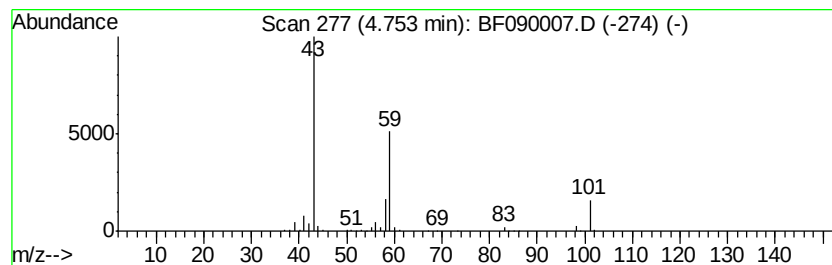
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.75	24.13 ng	1360600	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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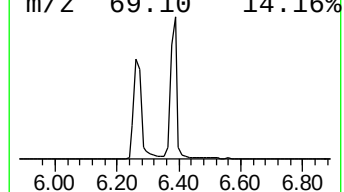
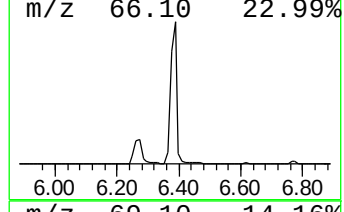
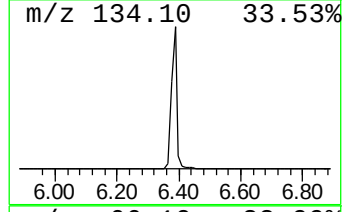
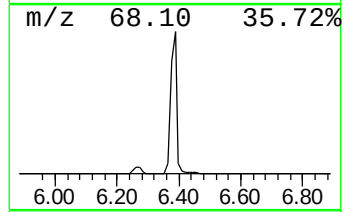
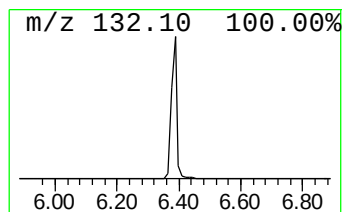
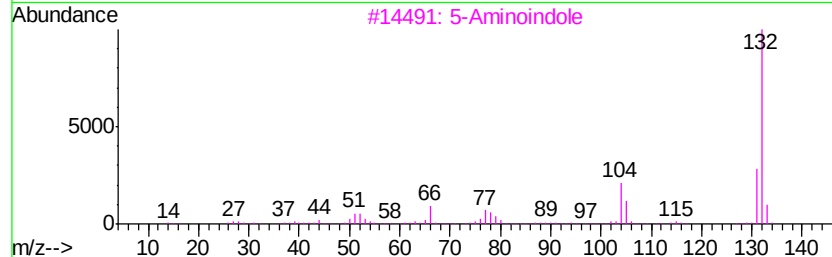
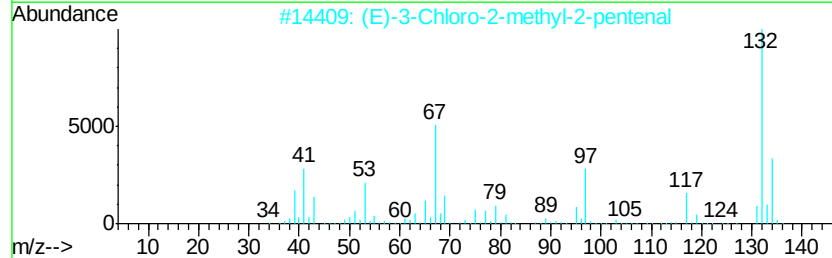
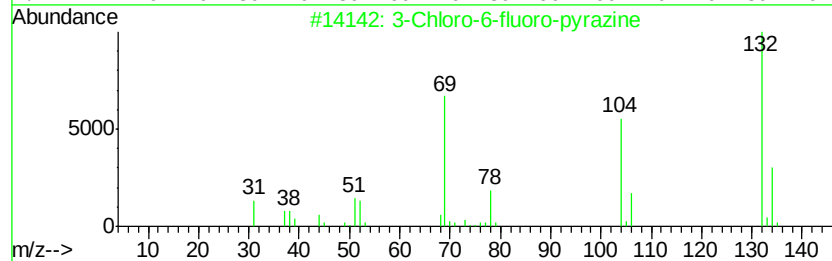
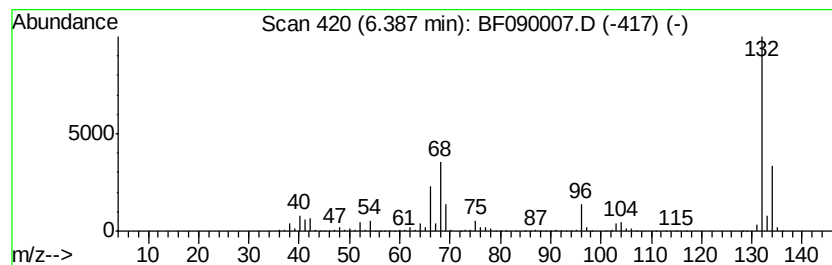
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Peak Number 3 unknown6.39 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	97.20 ng	5481330	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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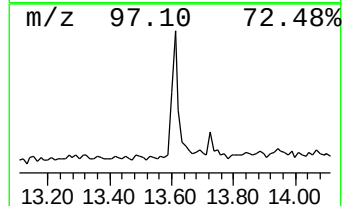
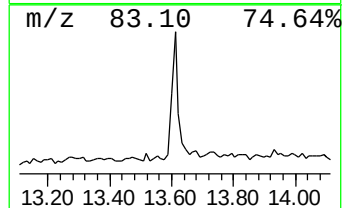
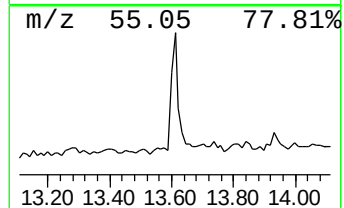
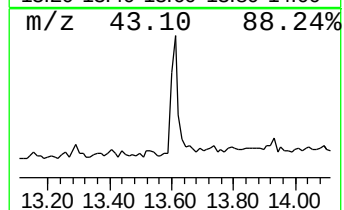
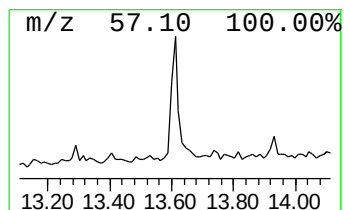
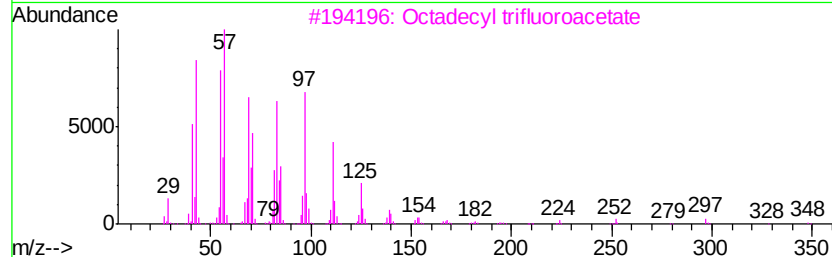
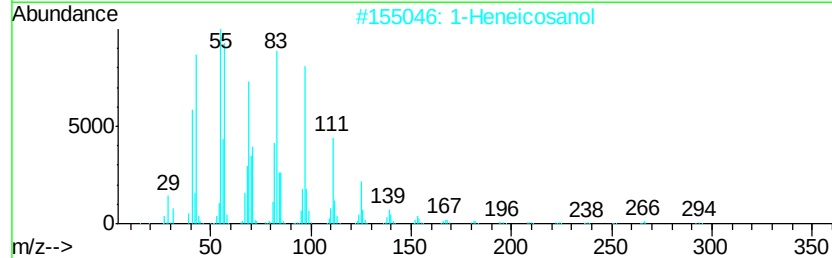
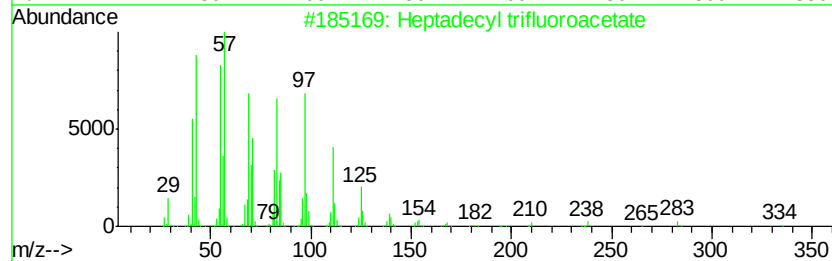
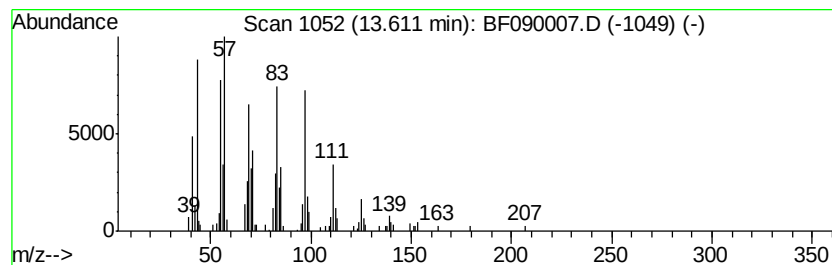
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Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.61	2.55 ng	185868	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	95
4		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5		Behenic alcohol	326	C22H46O	000661-19-8	94



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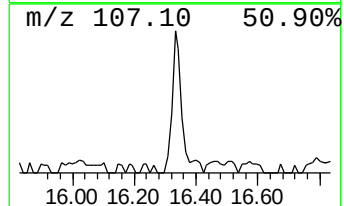
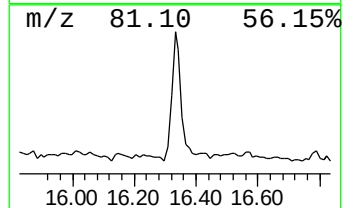
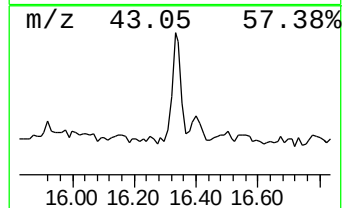
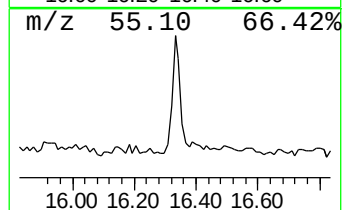
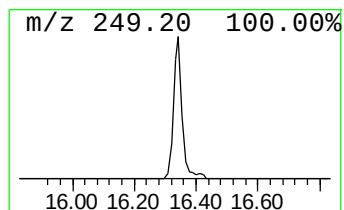
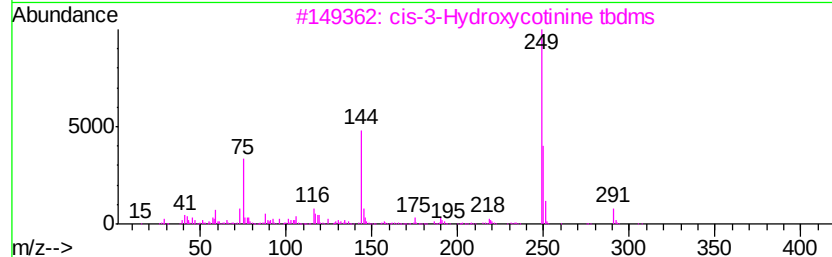
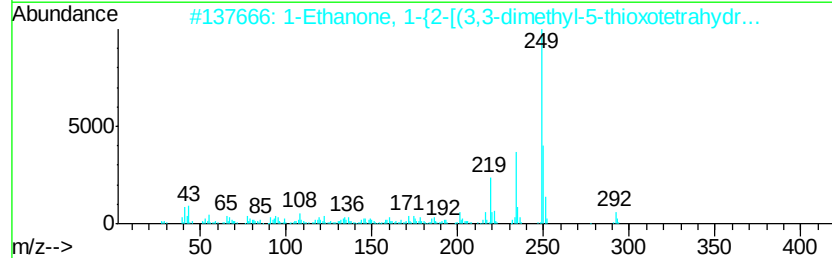
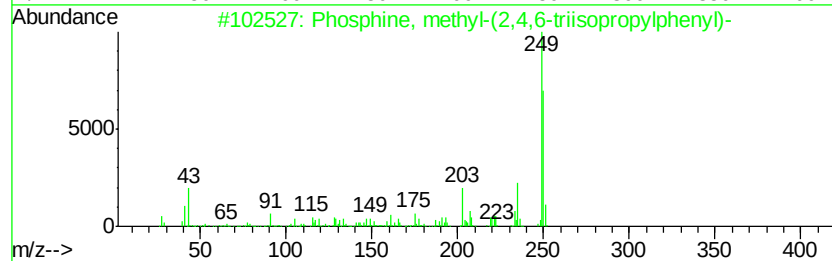
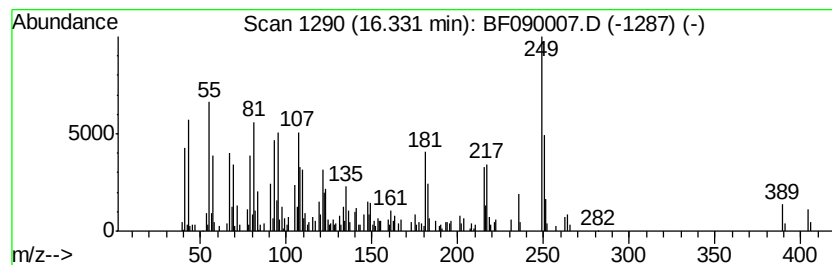
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Peak Number 6 Phosphine, methyl-(2,4,6-tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.33	6.77 ng	377348	Perylene-d12	15.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Phosphine, methyl-(2,4,6-triisop...	250 C16H27P	158748-69-7 50
2		1-Ethanone, 1-{2-[(3,3-dimethyl-...	292 C16H24N2OS	077109-20-7 32
3		cis-3-Hydroxycotinine tbdms	306 C16H26N2O2Si	1000331-70-7 25
4		Acetyl-1-(3-n-propoxyphenyl)-2-p...	249 C14H19NO3	1000122-90-2 25
5		12H-Benzo[a]phenothiazine	249 C16H11NS	000225-83-2 22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.75	24.1	ng	1360600	1	6.62	1127810	20.0
unknown6.39	6.39	97.2	ng	5481330	1	6.62	1127810	20.0
Heptadecyl triflu...	13.61	2.5	ng	185868	5	13.73	1460410	20.0
Phosphine, methyl...	16.33	6.8	ng	377348	6	15.06	1115560	20.0