

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080216\
 Data File : BF089553.D
 Acq On : 2 Aug 2016 18:11
 Operator : UM/SJ
 Sample : H4269-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-53-19.0-20.0

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-BF072716.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	1.644	4	5	42	rVB	671168	1420811	100.00%	12.687%
2	4.559	257	260	272	rBV	252539	408943	28.78%	3.652%
3	5.039	300	302	322	rBV	906169	1087344	76.53%	9.709%
4	5.450	336	338	345	rVB	16435	20422	1.44%	0.182%
5	6.136	395	398	405	rBV	991636	1202778	84.65%	10.740%
6	6.239	405	407	409	rBV	1146033	1149442	80.90%	10.264%
7	6.467	426	427	438	rVB3	182582	223445	15.73%	1.995%
8	6.627	438	441	443	rBV	663854	800698	56.35%	7.150%
9	7.050	476	478	502	rBV	422287	719362	50.63%	6.423%
10	7.759	538	540	552	rBV	268378	291594	20.52%	2.604%
11	8.833	632	634	637	rBV	1079009	1067422	75.13%	9.531%
12	9.233	667	669	672	rBV	162352	164744	11.60%	1.471%
13	9.496	690	692	695	rBV	370934	327004	23.02%	2.920%
14	9.953	730	732	734	rBV	21307	17080	1.20%	0.153%
15	10.285	759	761	771	rVV	651830	674448	47.47%	6.022%
16	10.422	771	773	780	rVB	26851	34346	2.42%	0.307%
17	10.971	819	821	826	rBV	271611	275300	19.38%	2.458%
18	12.548	957	959	962	rBV	882416	847602	59.66%	7.569%
19	13.474	1038	1040	1045	rBB	26817	43254	3.04%	0.386%
20	13.588	1048	1050	1058	rBV	213499	224095	15.77%	2.001%
21	14.914	1163	1166	1169	rBV	180337	198858	14.00%	1.776%

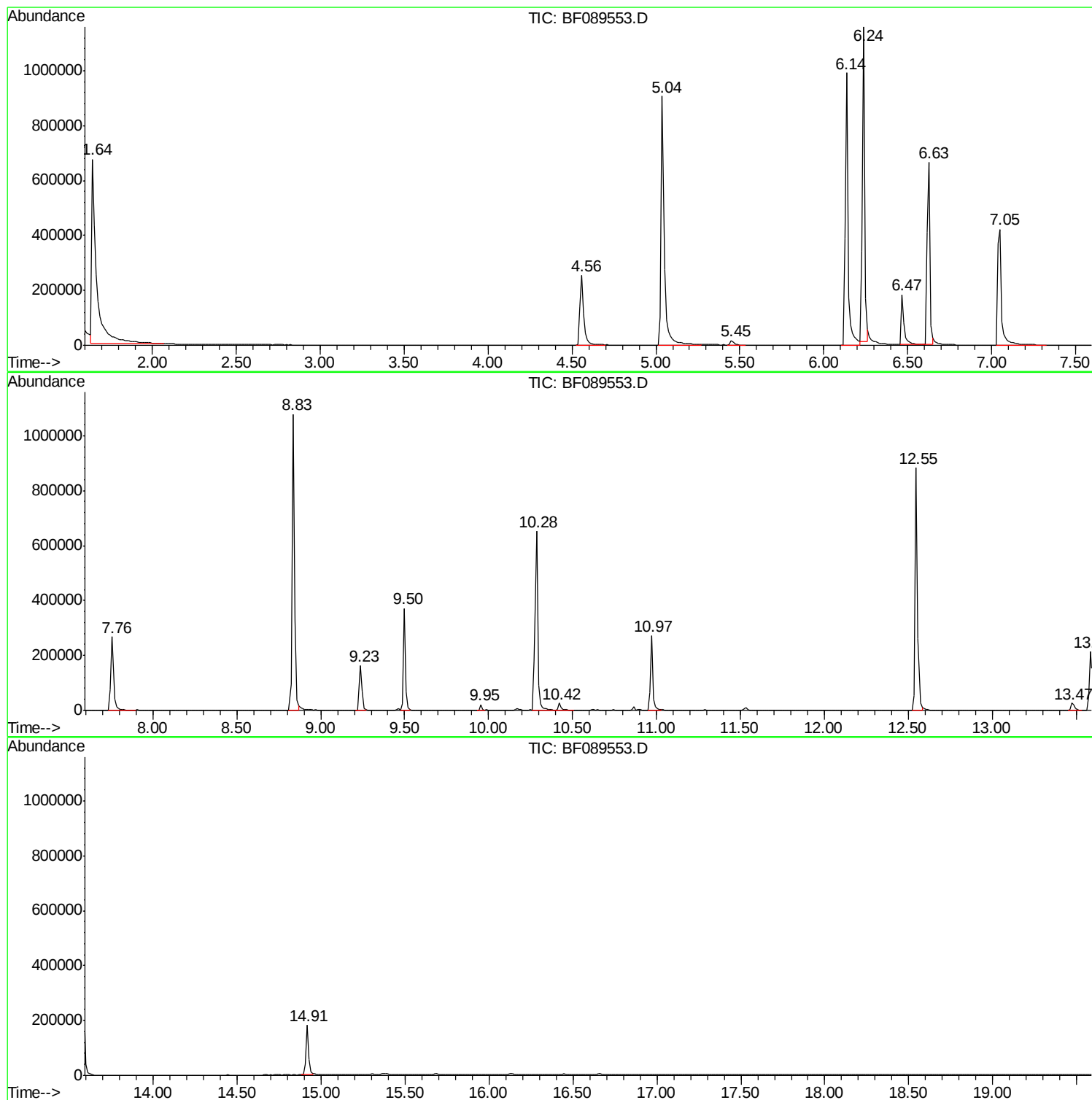
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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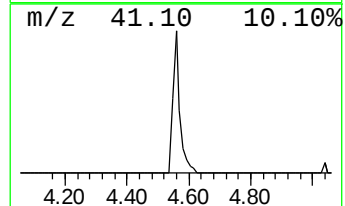
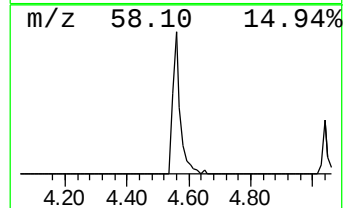
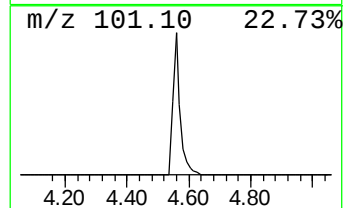
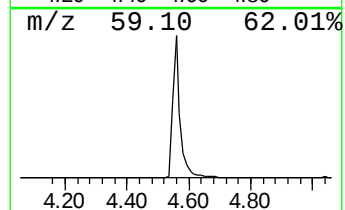
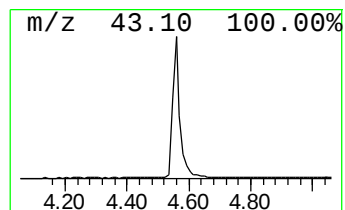
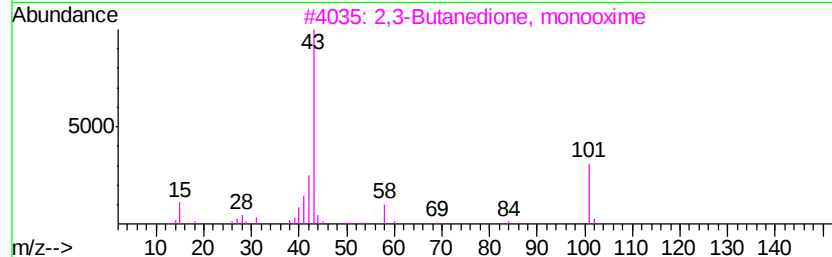
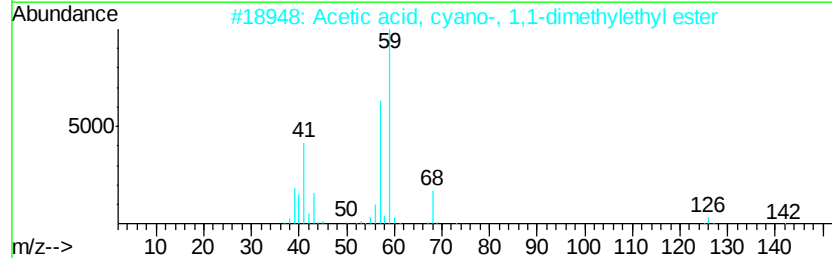
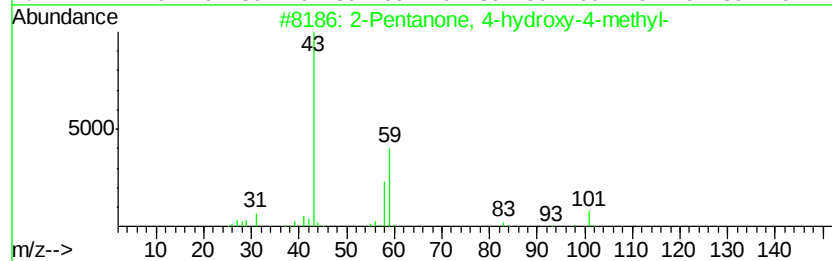
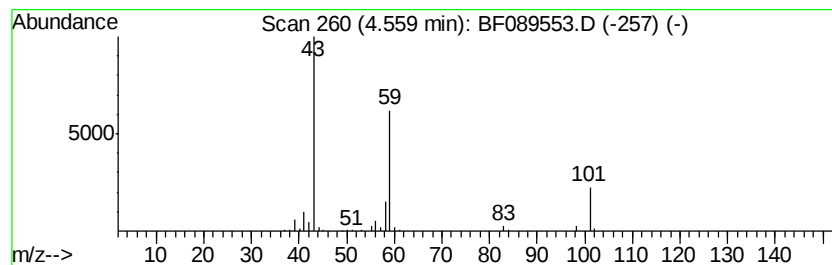
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.56	36.60 ng	408943	1,4-Dichlorobenzene-d4	6.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
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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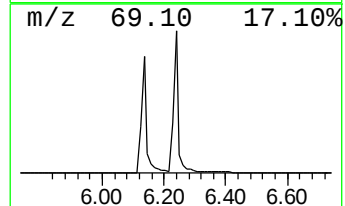
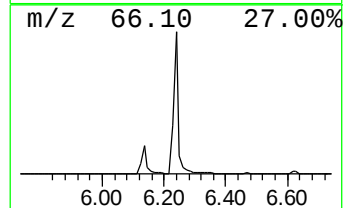
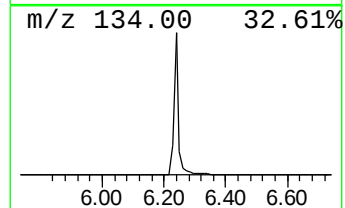
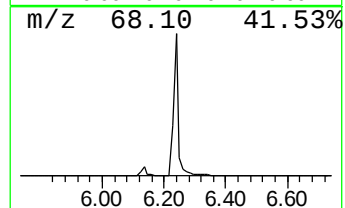
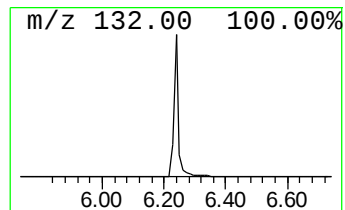
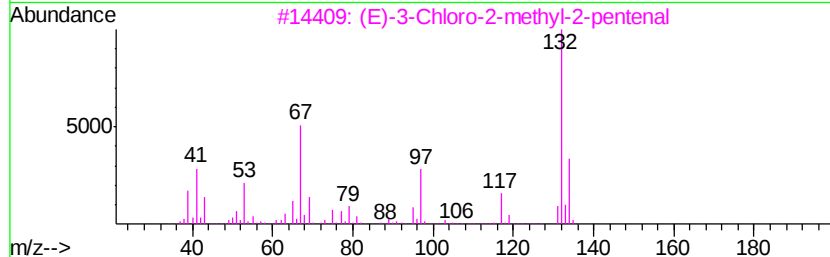
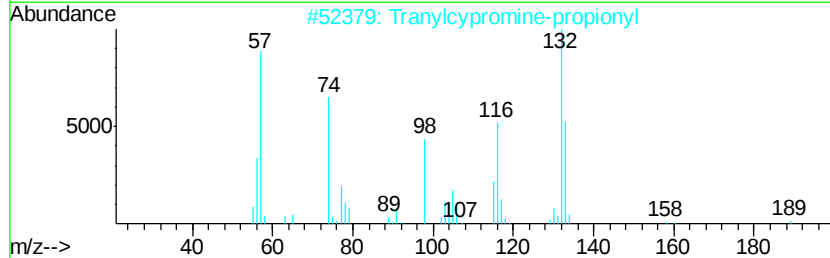
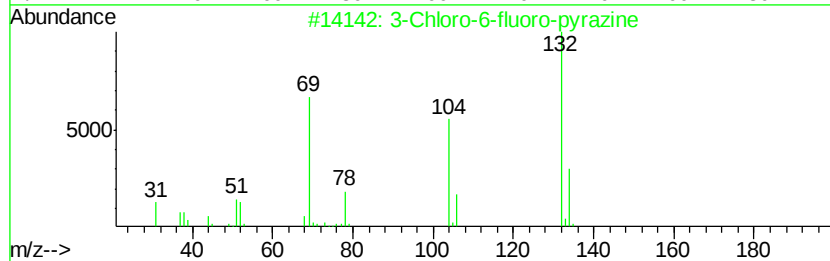
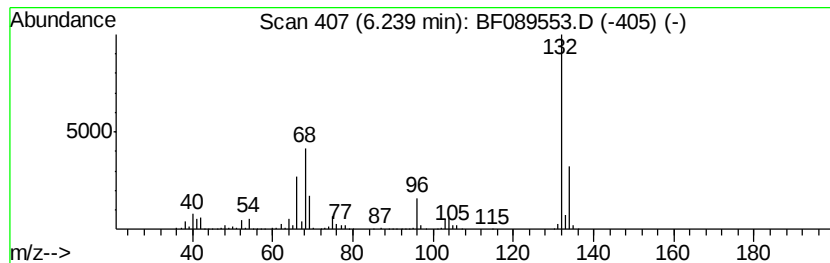
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Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	102.88 ng	1149440	1,4-Dichlorobenzene-d4	6.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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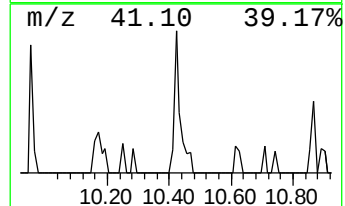
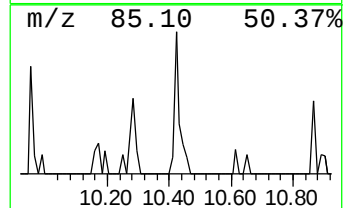
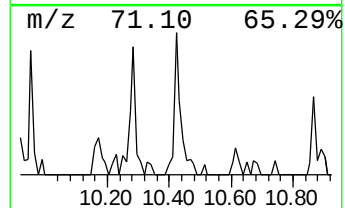
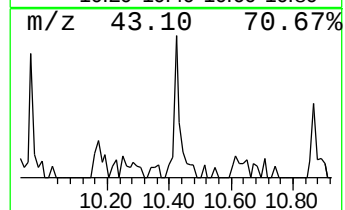
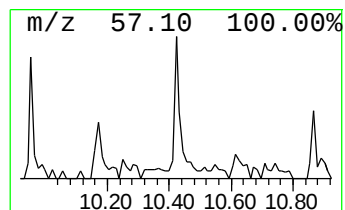
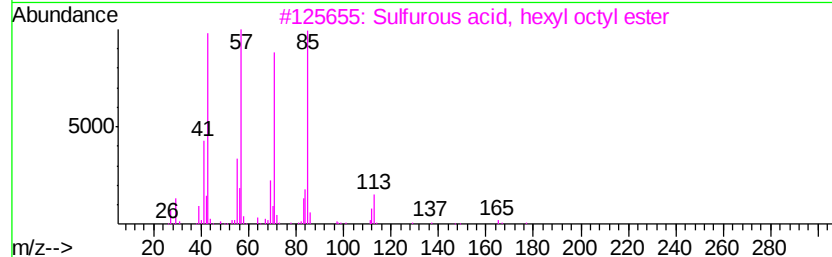
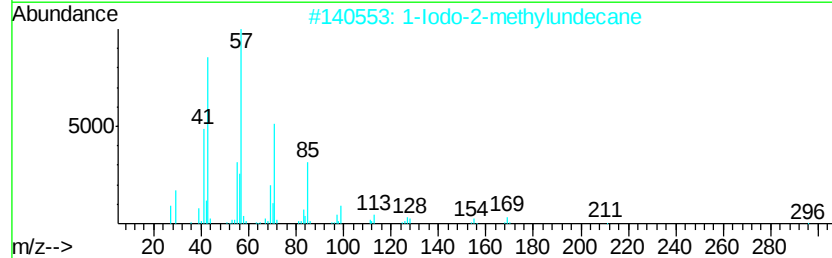
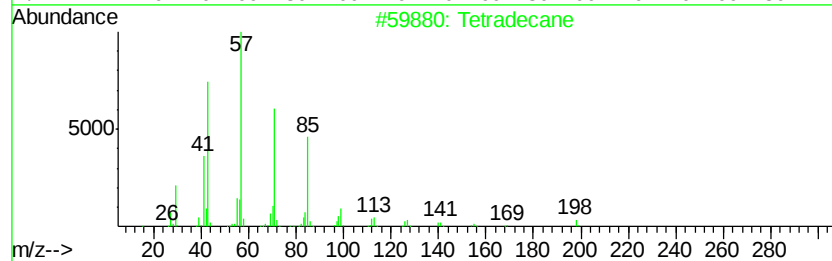
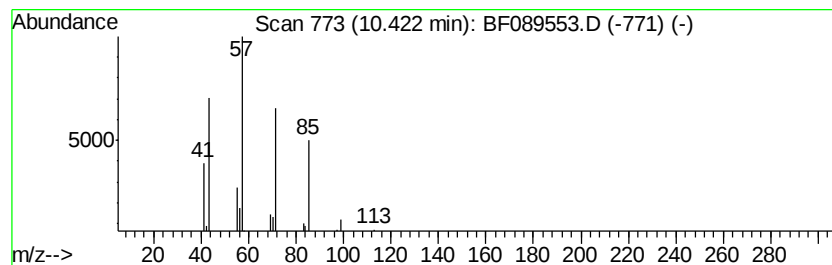
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Peak Number 5 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.42	2.50 ng	34346	Phenanthrene-d10	10.97	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	64
2	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
3	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59
4	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59
5	Sulfurous acid, 2-ethylhexyl hep...	432	C25H52O3S	1000309-20-0	53



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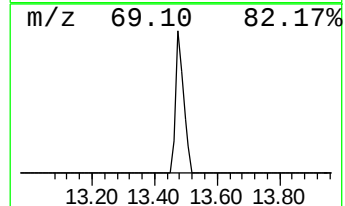
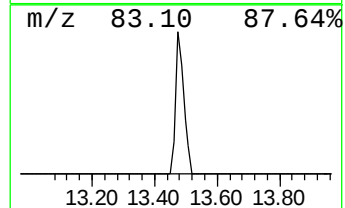
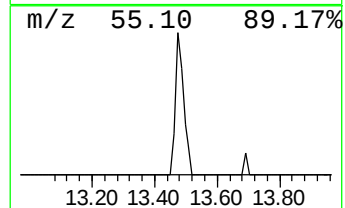
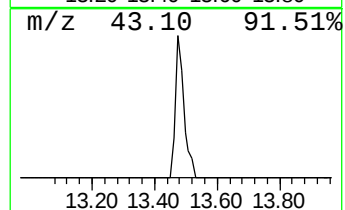
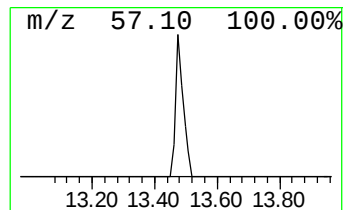
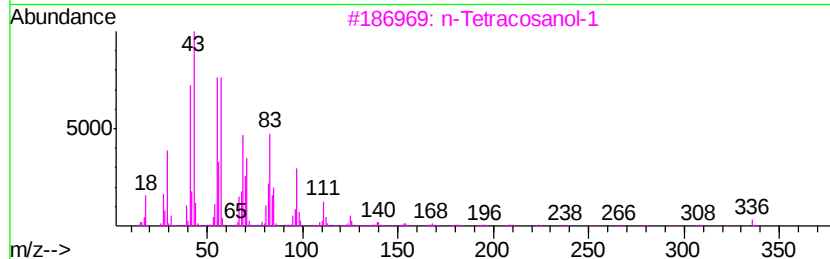
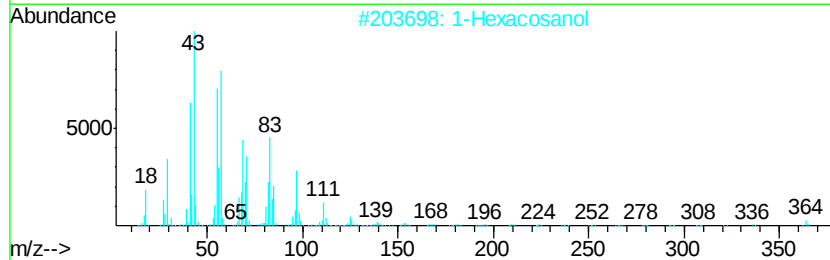
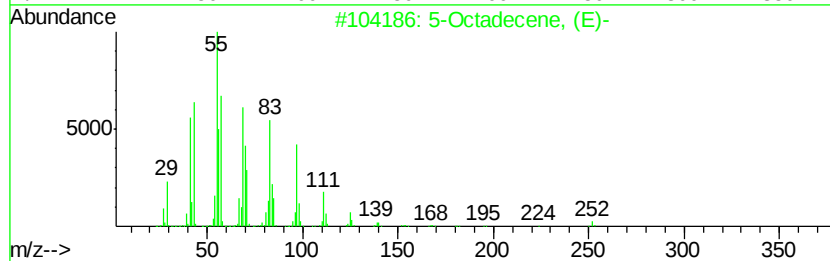
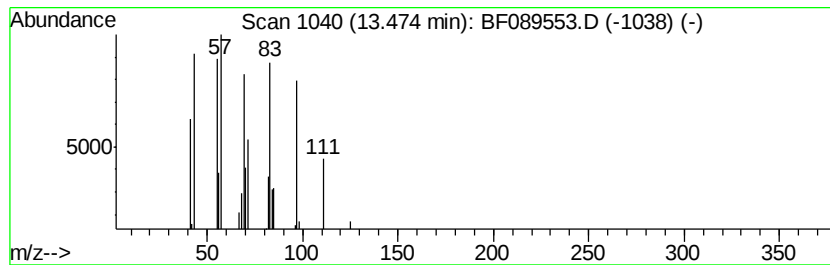
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Peak Number 6 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	3.86 ng	43254	Chrysene-d12	13.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Octadecene, (E)-	252	C18H36	007206-21-5	59
2		1-Hexacosanol	382	C26H54O	000506-52-5	52
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	52
4		Carbonic acid, isobutyl octadecyl ester	370	C23H46O3	1000314-61-5	50
5		Oxalic acid, allyl dodecyl ester	298	C17H30O4	1000309-24-0	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.56	36.6	ng	408943	1	6.47	223445	20.0
unknown6.24	6.24	102.9	ng	1149440	1	6.47	223445	20.0
Tetradecane	10.42	2.5	ng	34346	4	10.97	275300	20.0
5-Octadecene, (E)-	13.47	3.9	ng	43254	5	13.59	224095	20.0