

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
 Data File : BF089652.D
 Acq On : 6 Aug 2016 5:51
 Operator : UM/SJ
 Sample : H4351-02
 Misc :
 ALS Vial : 54 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CORE-E

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-BF080416.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	4.661	266	269	289	rVB	135942	372741	22.84%	3.091%
2	5.336	326	328	354	rBV	762165	1441409	88.32%	11.953%
3	6.982	469	472	479	rBV	782493	1430852	87.67%	11.866%
4	7.096	479	482	502	rVB	1112214	1632045	100.00%	13.534%
5	7.439	510	512	523	rBV	132404	229871	14.08%	1.906%
6	7.679	530	533	547	rBV	907864	1162388	71.22%	9.639%
7	8.353	589	592	616	rBV	549151	903533	55.36%	7.493%
8	9.473	687	690	705	rBV	181622	311722	19.10%	2.585%
9	11.256	842	846	848	rBV	1090775	1593845	97.66%	13.217%
10	11.942	903	906	912	rBV	140066	213580	13.09%	1.771%
11	12.285	934	936	939	rBV	204107	310177	19.01%	2.572%
12	12.331	939	940	947	rVB	16539	21709	1.33%	0.180%
13	13.154	1009	1012	1014	rVB	21741	29842	1.83%	0.247%
14	13.508	1039	1043	1047	rBV	6821	16603	1.02%	0.138%
15	13.577	1047	1049	1058	rBV	450721	669905	41.05%	5.555%
16	13.919	1076	1079	1084	rBV	26343	39542	2.42%	0.328%
17	14.685	1144	1146	1153	rVB	170700	229395	14.06%	1.902%
18	17.051	1350	1353	1356	rBV	817815	956233	58.59%	7.930%
19	18.308	1461	1463	1467	rBV	31581	57347	3.51%	0.476%
20	18.377	1467	1469	1481	rVB	137685	218794	13.41%	1.814%
21	19.543	1568	1571	1573	rBV	28479	32490	1.99%	0.269%
22	20.046	1613	1615	1621	rBV	145718	184607	11.31%	1.531%

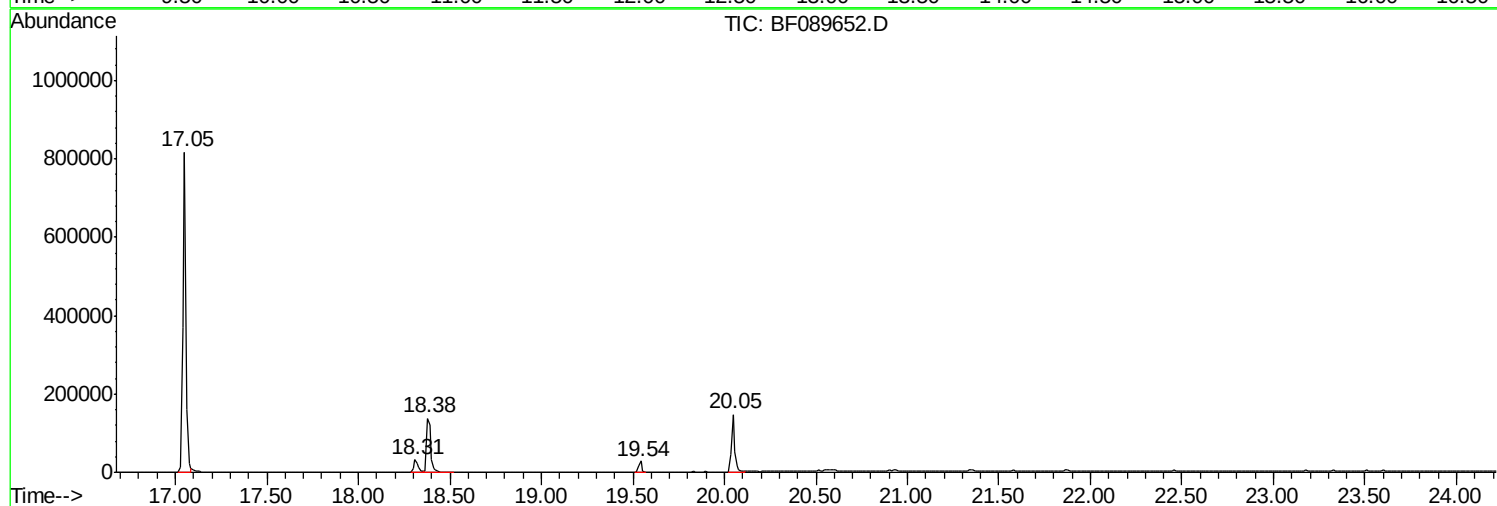
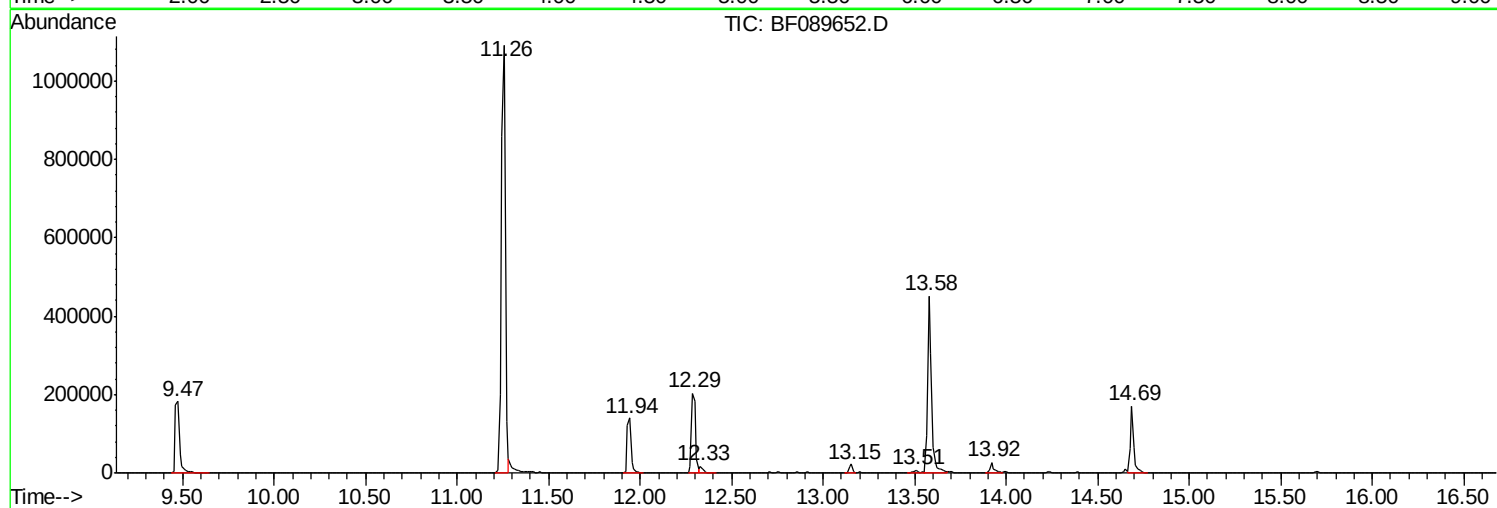
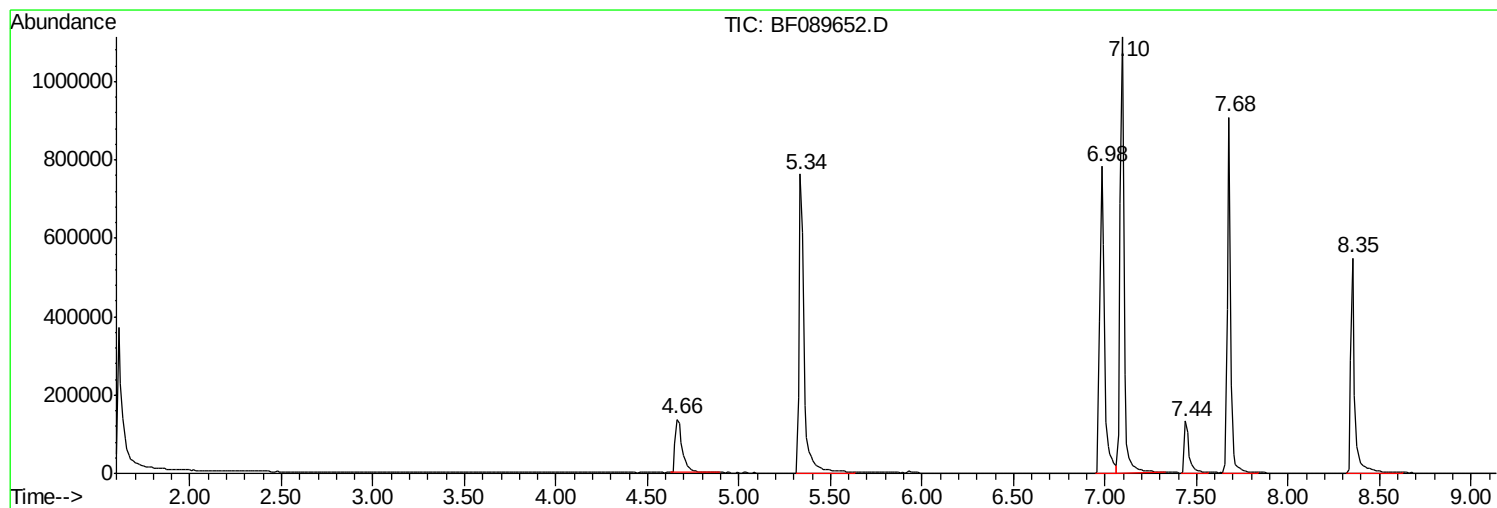
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 6 Aug 2016 5:51
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Instrument :
BNA_F
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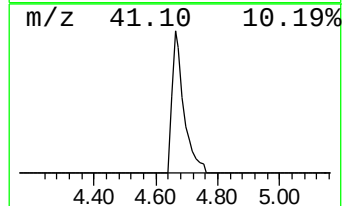
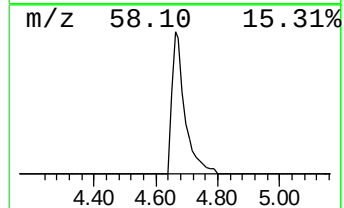
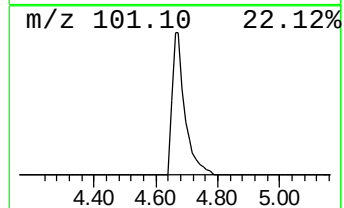
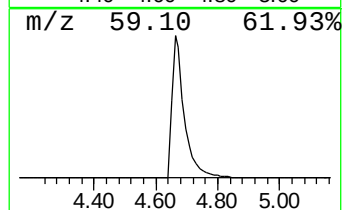
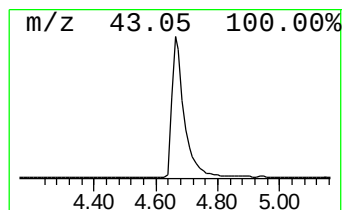
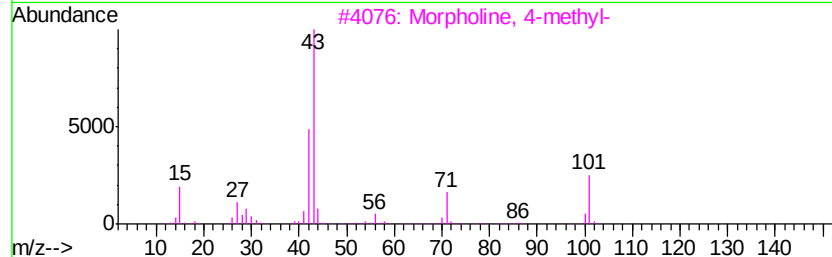
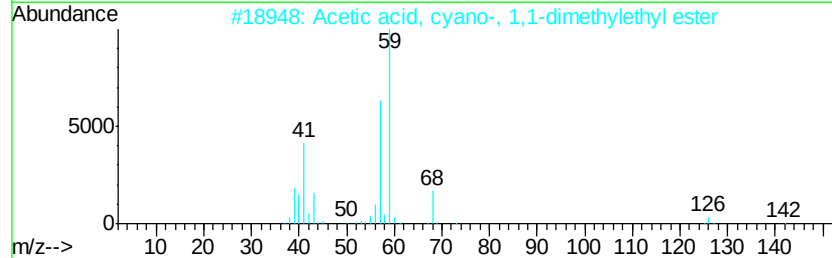
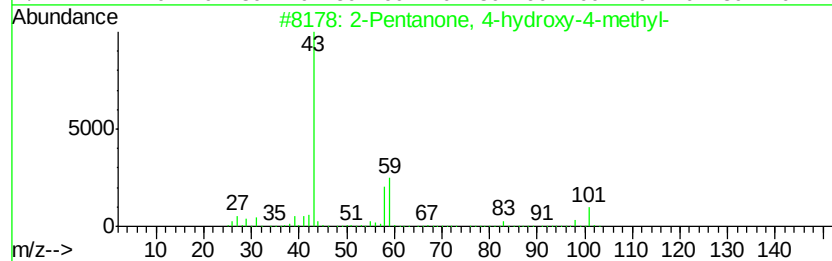
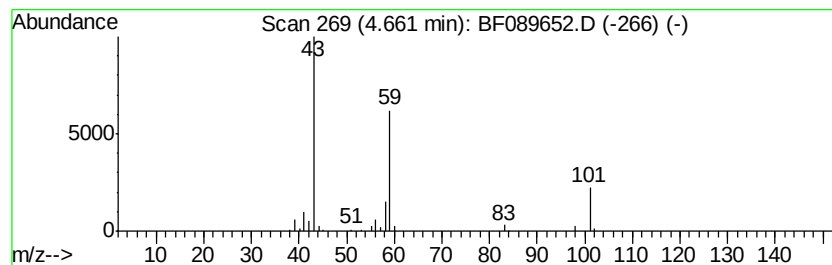
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.66	32.43 ng	372741	1,4-Dichlorobenzene-d4	7.44

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-dimethy...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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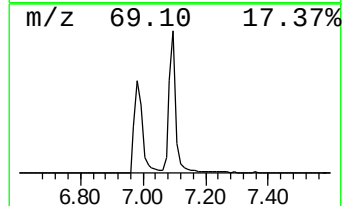
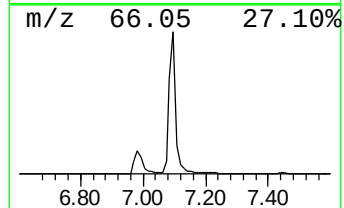
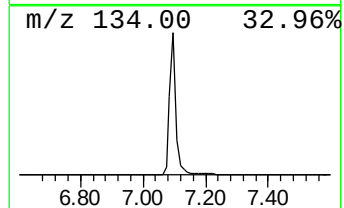
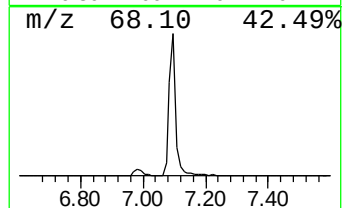
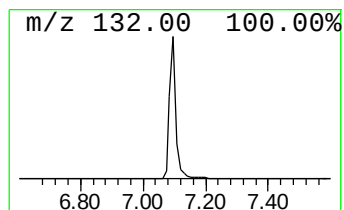
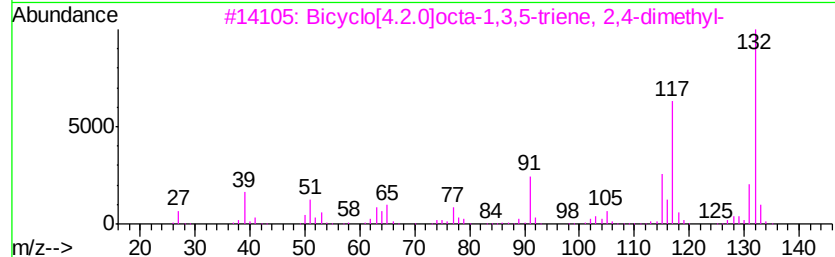
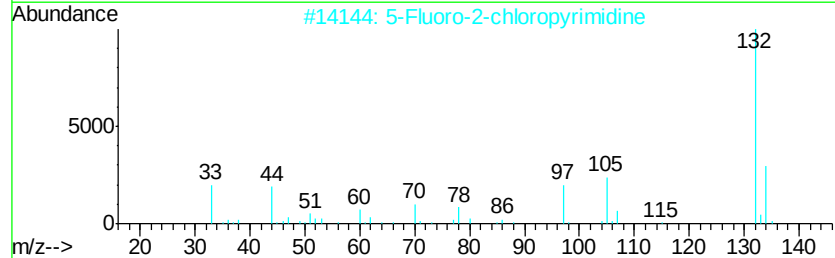
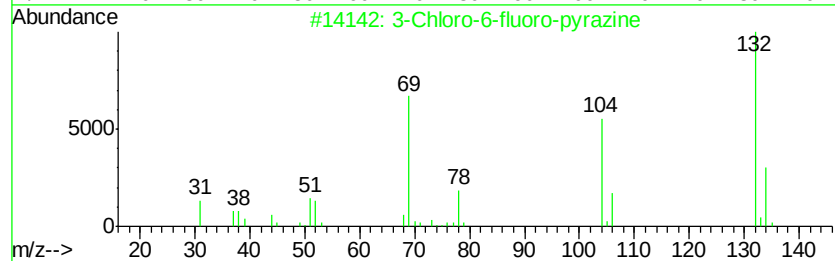
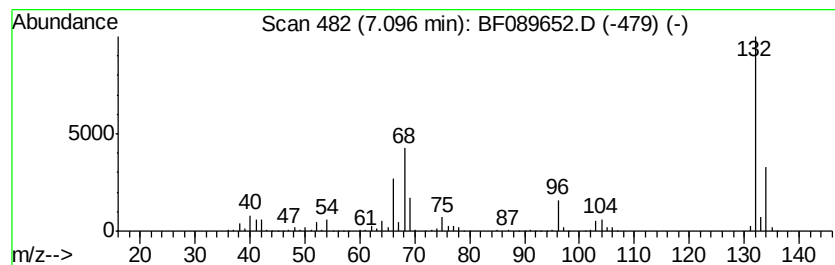
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Peak Number 2 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	142.00 ng	1632050	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		Xenon	132	Xe	007440-63-3	9



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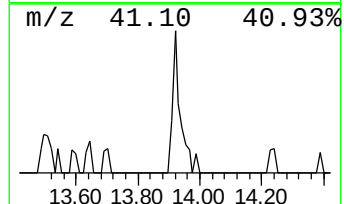
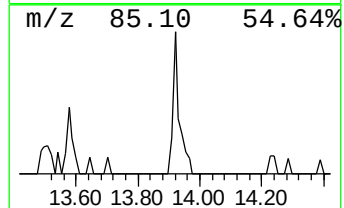
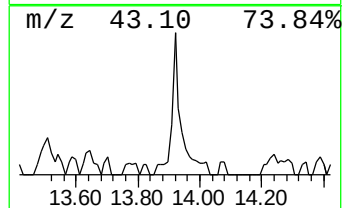
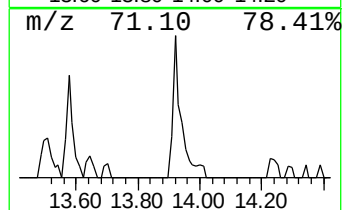
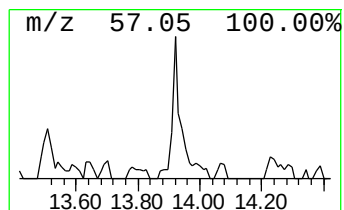
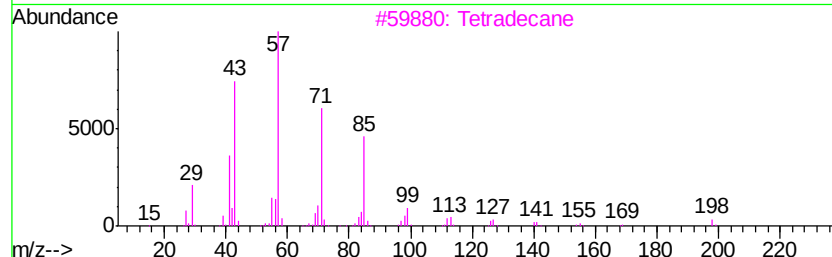
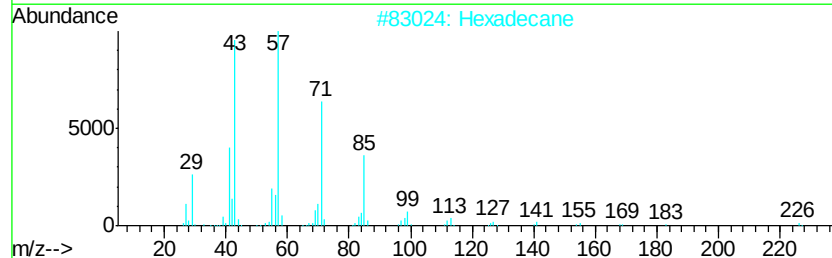
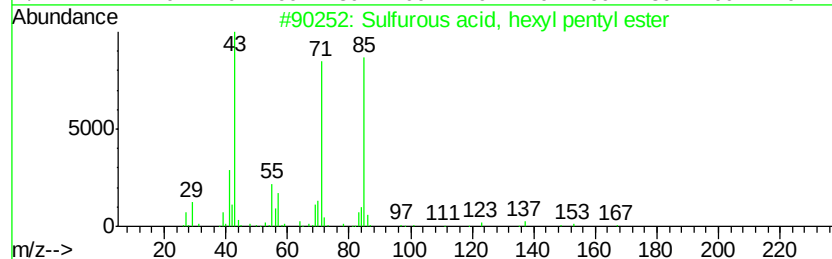
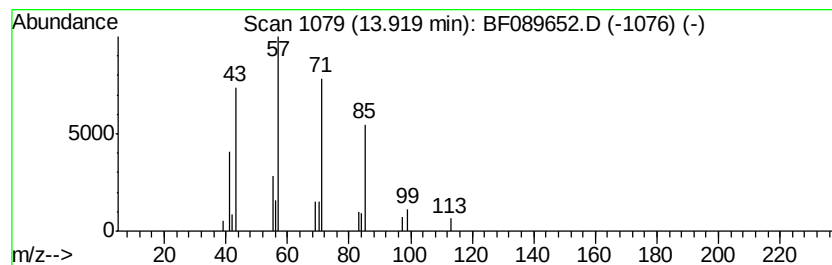
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Peak Number 4 Sulfurous acid, hexyl penty... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.45 ng	39542	Phenanthrene-d10	14.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	80
2		Hexadecane	226	C16H34	000544-76-3	72
3		Tetradecane	198	C14H30	000629-59-4	72
4		Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	64
5		Sulfurous acid, 2-ethylhexyl hex...	418	C24H50O3S	1000309-19-9	59



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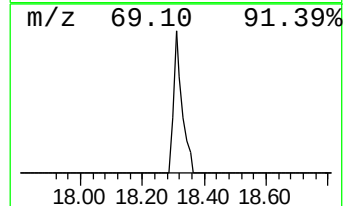
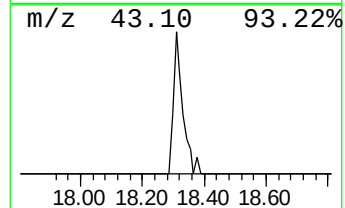
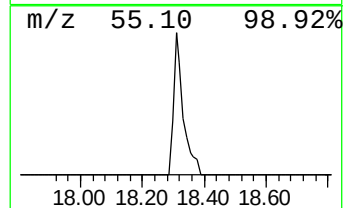
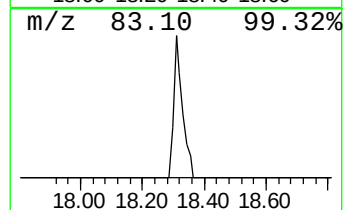
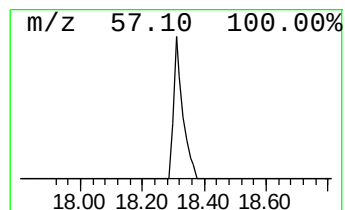
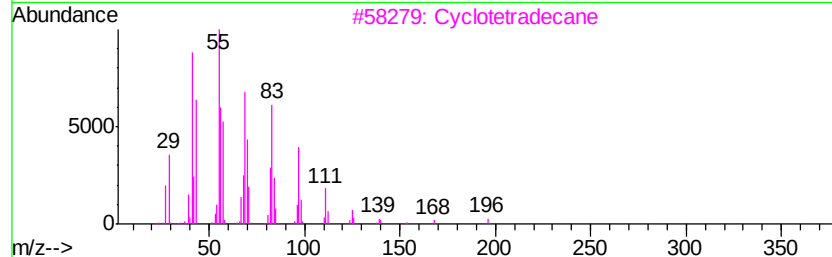
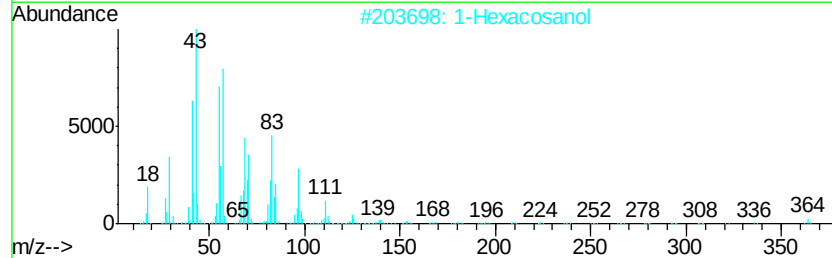
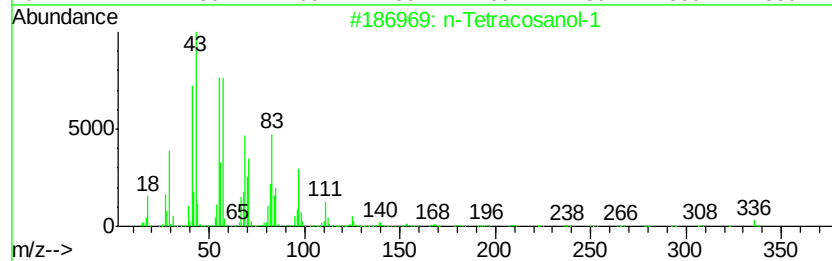
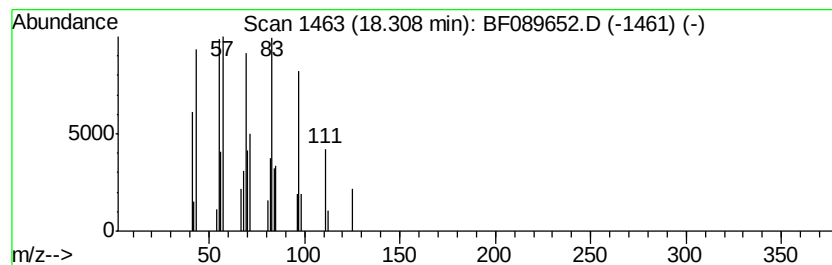
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	5.24 ng	57347	Chrysene-d12	18.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	58
2		1-Hexacosanol	382	C26H54O	000506-52-5	52
3		Cyclotetradecane	196	C14H28	000295-17-0	43
4		Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	43
5		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	38



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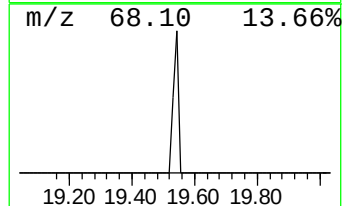
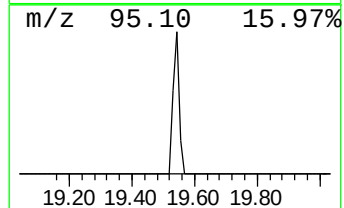
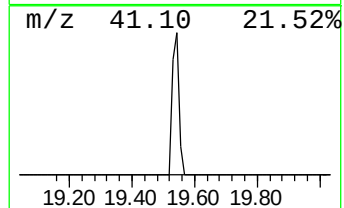
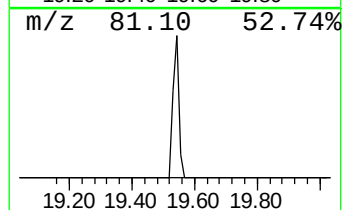
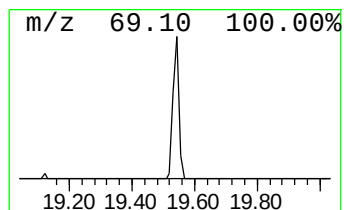
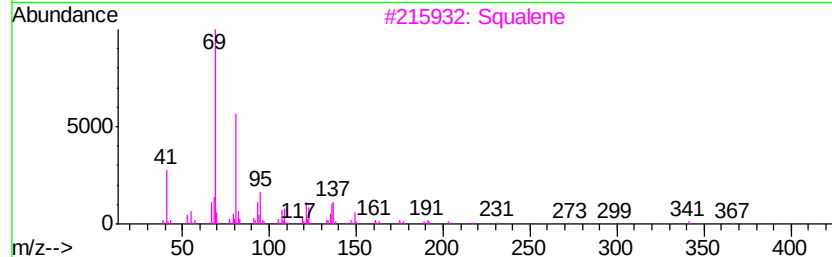
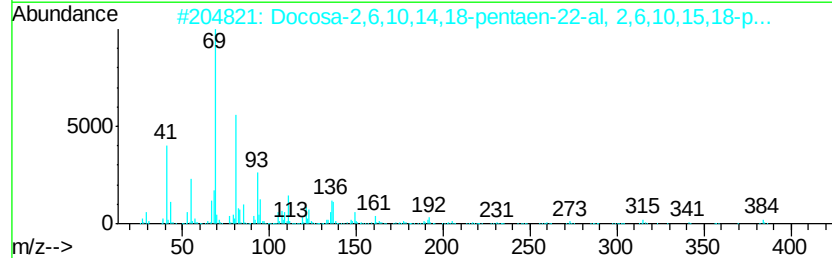
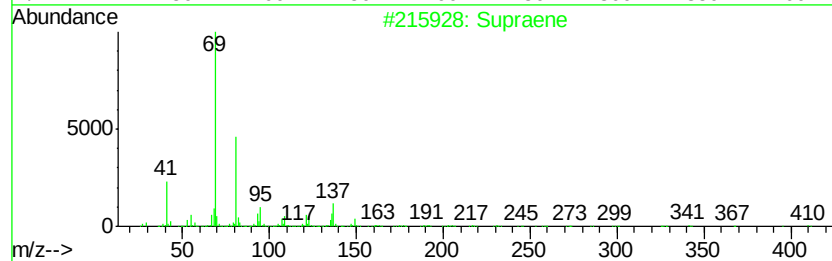
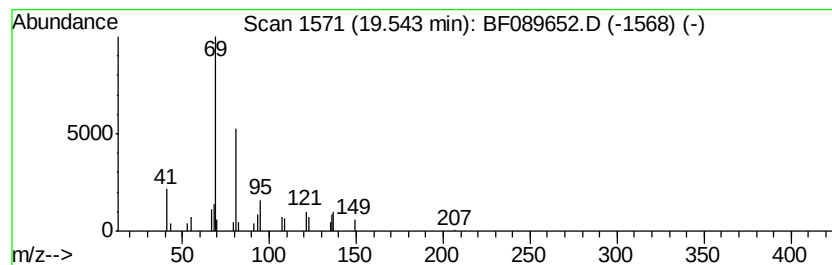
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Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.54	3.52 ng	32490	Perylene-d12	20.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	90
2	Docosa-2,6,10,14,18-pentaen-22-a...		384	C27H44O	1000163-04-7	90
3	Squalene		410	C30H50	000111-02-4	90
4	.psi.,.psi.-Carotene, 7,7',8,8',...		547	C40H66	000502-62-5	83
5	Hexadeca-2,6,10,14-tetraen-1-ol,...		290	C20H34O	007614-21-3	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.66	32.4	ng	372741	1	7.44	229871	20.0
unknown7.10	7.10	142.0	ng	1632050	1	7.44	229871	20.0
Sulfurous acid, h...	13.92	3.5	ng	39542	4	14.69	229395	20.0
n-Tetracosanol-1	18.31	5.2	ng	57347	5	18.39	218794	20.0
Supraene	19.54	3.5	ng	32490	6	20.05	184607	20.0