

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080516\
Data File : BF089651.D
Acq On : 6 Aug 2016 5:17
Operator : UM/SJ
Sample : H4351-01
Misc :
ALS Vial : 53 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-4

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-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	281	rBV	122487	296050	22.01%	2.909%
2	5.336	326	328	355	rBV	694956	1155606	85.92%	11.354%
3	6.982	469	472	479	rBV	731233	1142376	84.93%	11.224%
4	7.096	479	482	504	rVB	803580	1345046	100.00%	13.216%
5	7.439	510	512	522	rBV	129538	219535	16.32%	2.157%
6	7.679	530	533	547	rBV	704142	966917	71.89%	9.500%
7	8.353	589	592	617	rBV	433464	743610	55.29%	7.306%
8	9.462	687	689	708	rBV	179519	306251	22.77%	3.009%
9	11.245	842	845	848	rBV	799854	1300346	96.68%	12.776%
10	11.942	903	906	912	rBV	140307	219014	16.28%	2.152%
11	12.285	934	936	939	rBV	192666	300251	22.32%	2.950%
12	12.331	939	940	943	rVB	12238	14372	1.07%	0.141%
13	13.154	1009	1012	1014	rBV	19420	25674	1.91%	0.252%
14	13.577	1047	1049	1054	rBV	389585	553044	41.12%	5.434%
15	13.919	1076	1079	1084	rBV	21856	34406	2.56%	0.338%
16	14.685	1144	1146	1154	rVB	158629	222728	16.56%	2.188%
17	17.051	1350	1353	1363	rBV	708910	839087	62.38%	8.244%
18	18.308	1461	1463	1467	rBV	20520	37540	2.79%	0.369%
19	18.388	1467	1470	1477	rVB	131526	214763	15.97%	2.110%
20	19.543	1569	1571	1573	rBV	43604	44731	3.33%	0.439%
21	20.046	1613	1615	1622	rBV	148329	196392	14.60%	1.930%

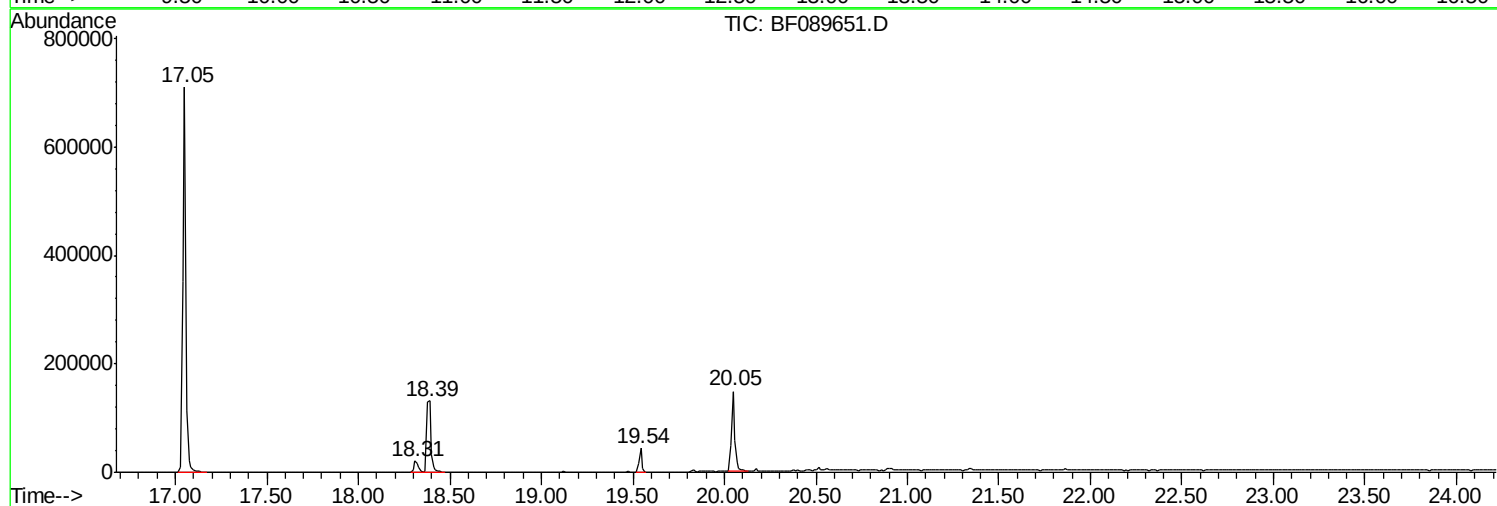
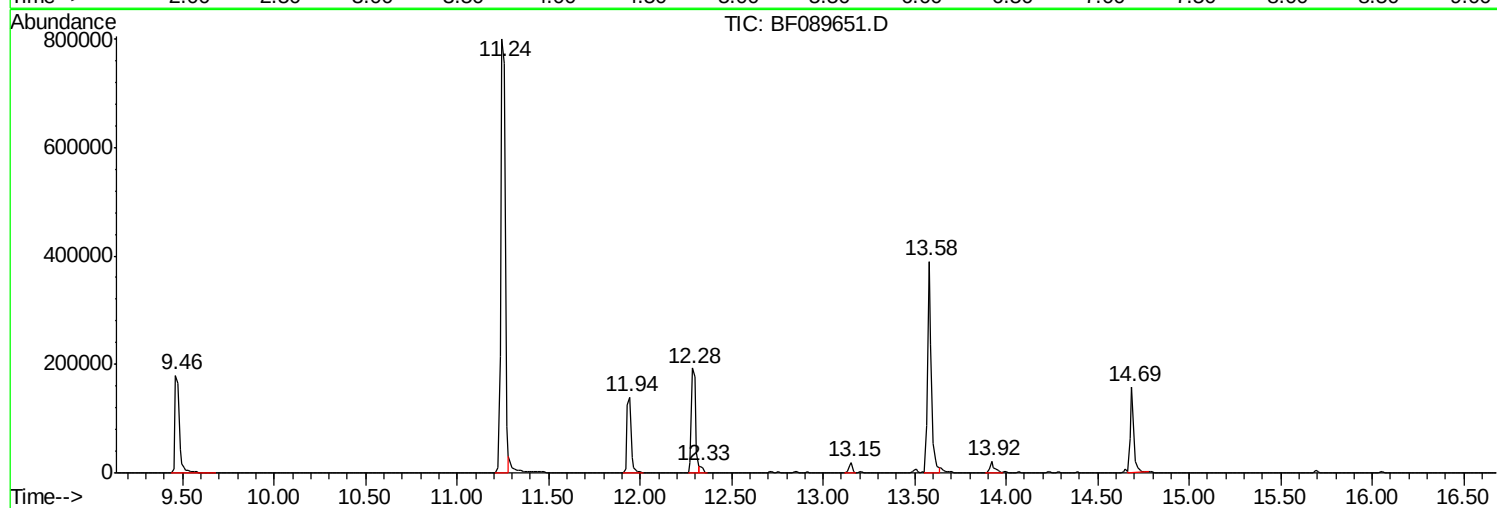
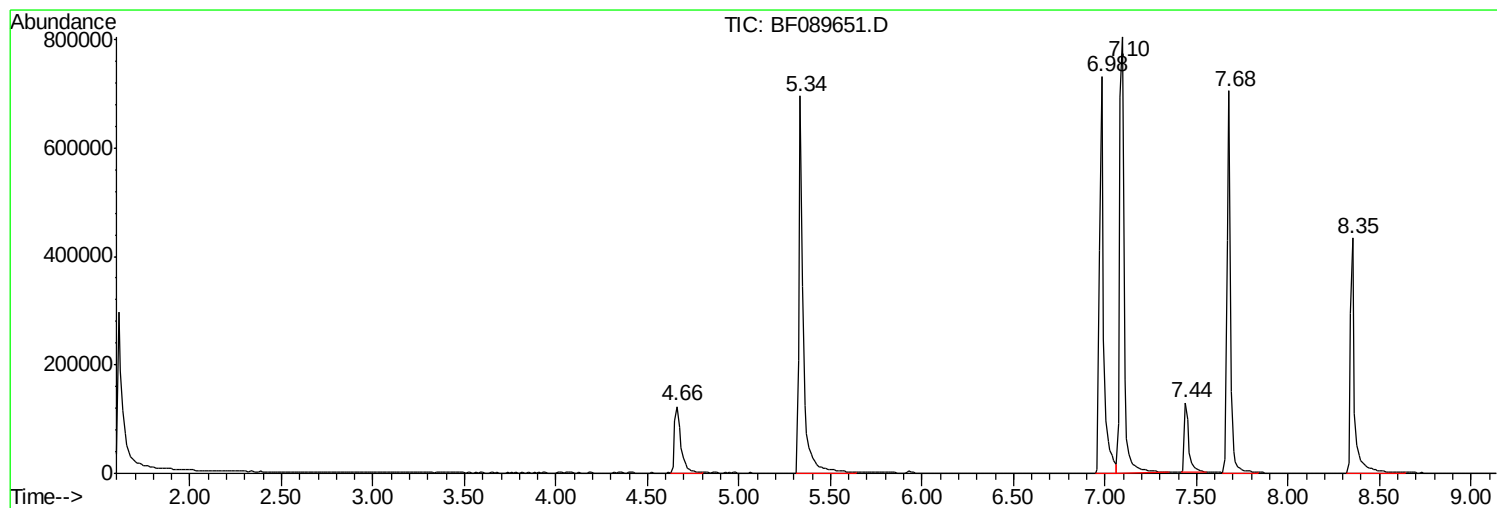
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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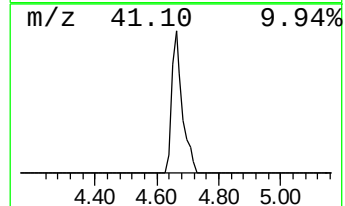
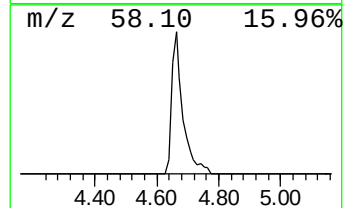
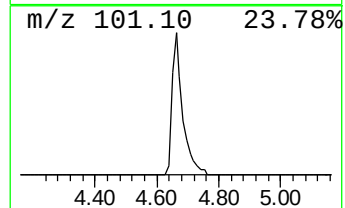
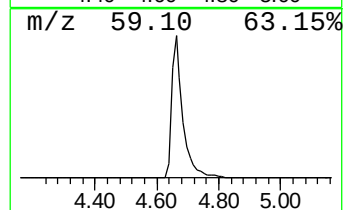
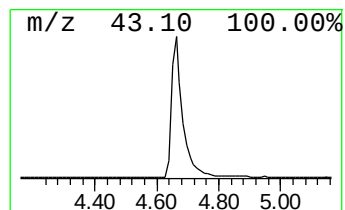
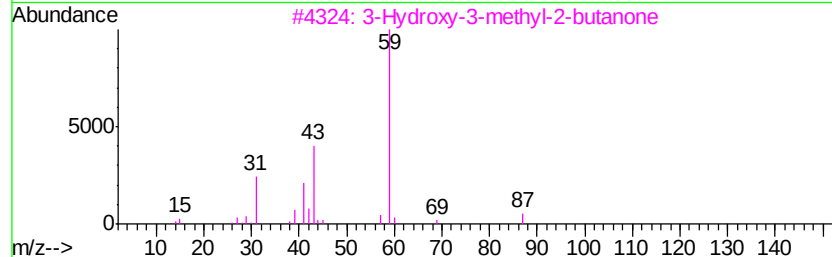
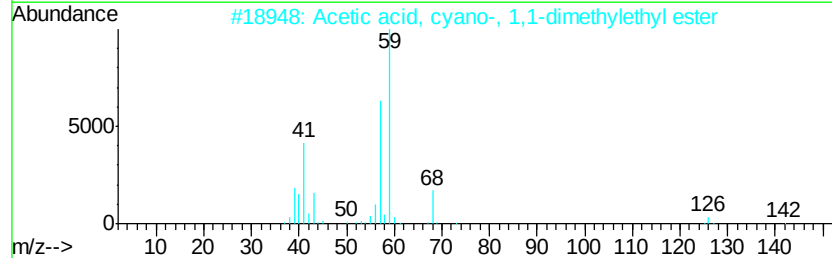
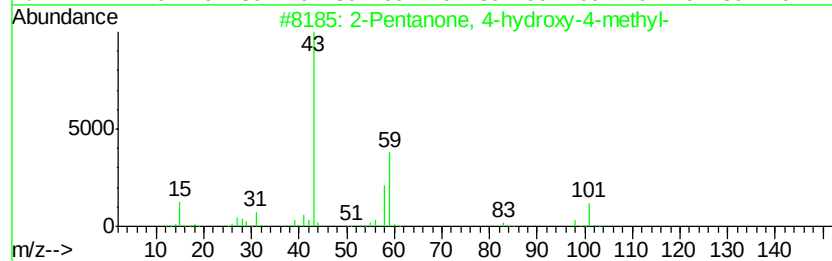
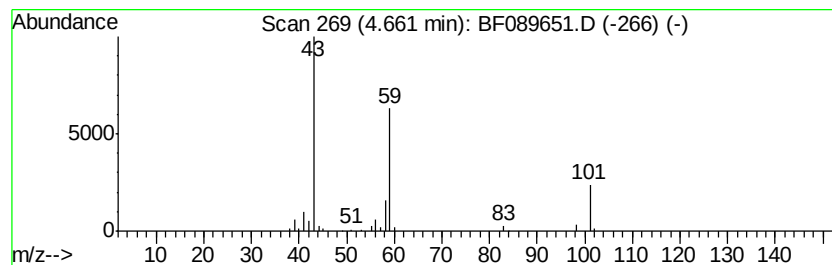
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	26.97 ng	296050	1,4-Dichlorobenzene-d4	7.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17	
4	Acetone	58	C3H6O	000067-64-1	10	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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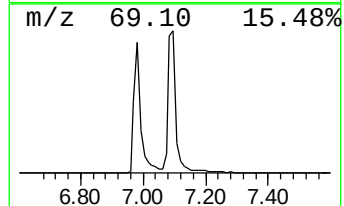
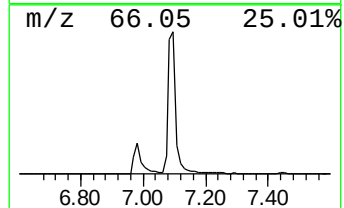
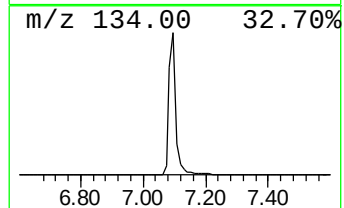
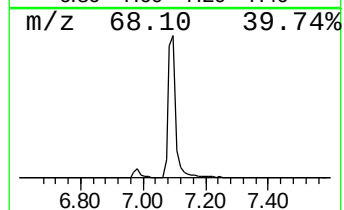
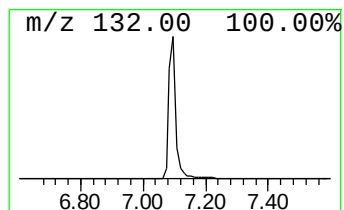
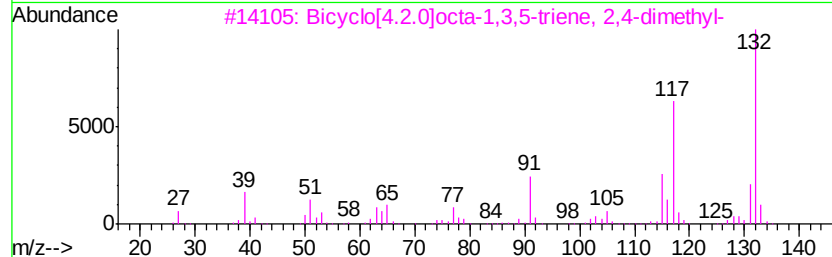
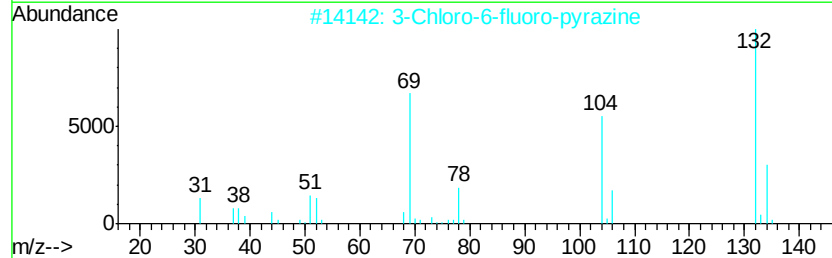
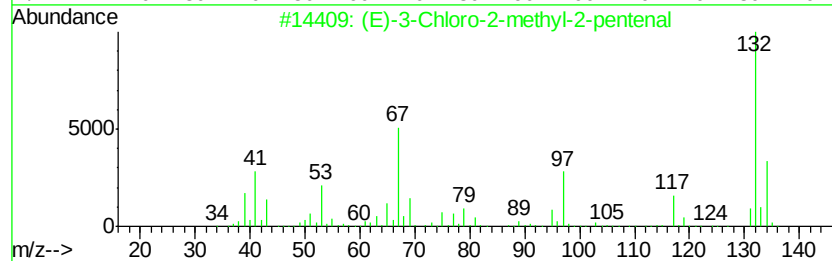
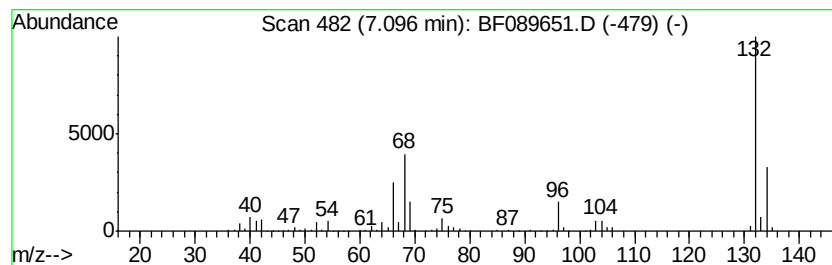
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Peak Number 2 unknown7.10 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	122.54 ng	1345050	1,4-Dichlorobenzene-d4	7.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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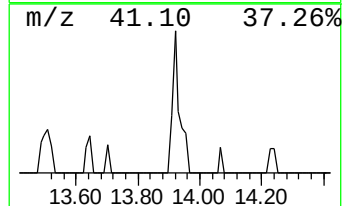
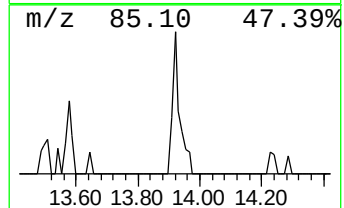
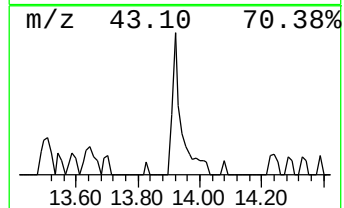
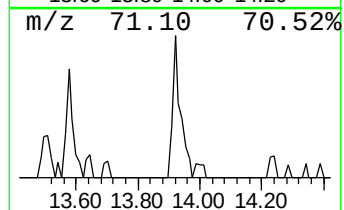
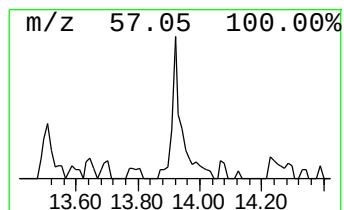
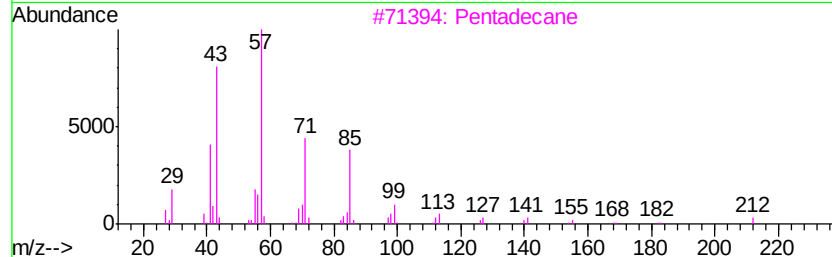
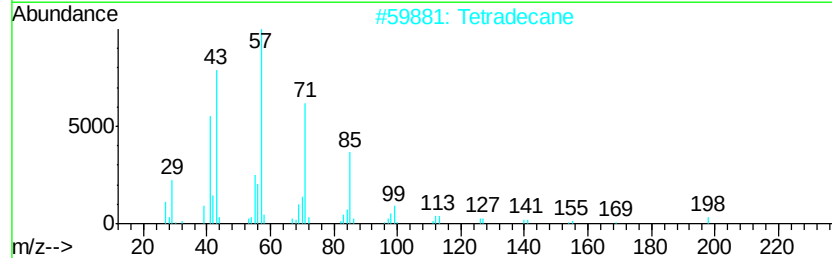
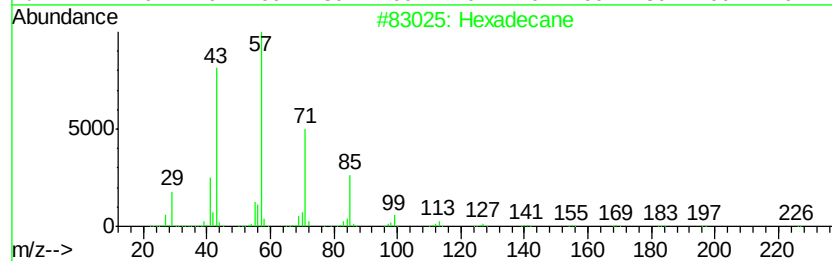
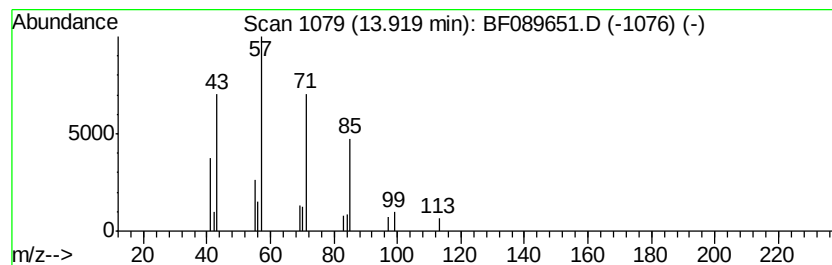
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Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	3.09 ng	34406	Phenanthrene-d10	14.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	83
2		Tetradecane	198	C14H30	000629-59-4	83
3		Pentadecane	212	C15H32	000629-62-9	78
4		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72
5		Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	72



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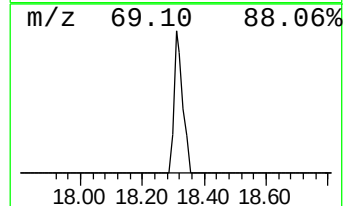
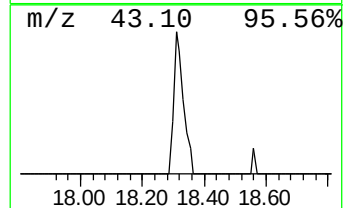
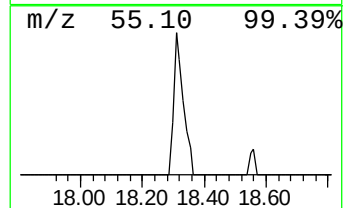
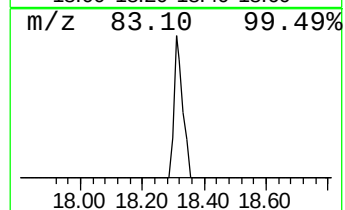
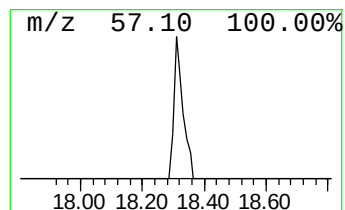
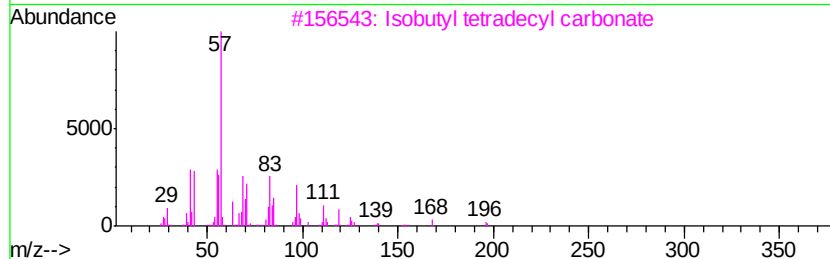
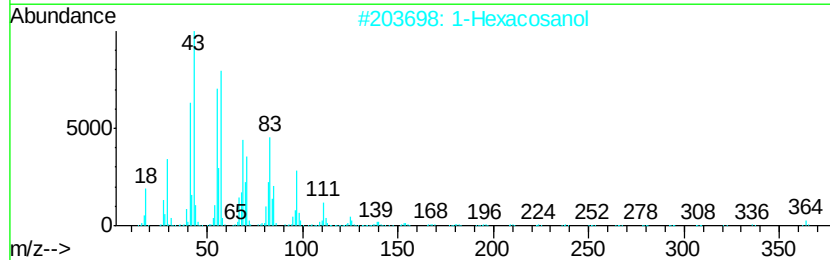
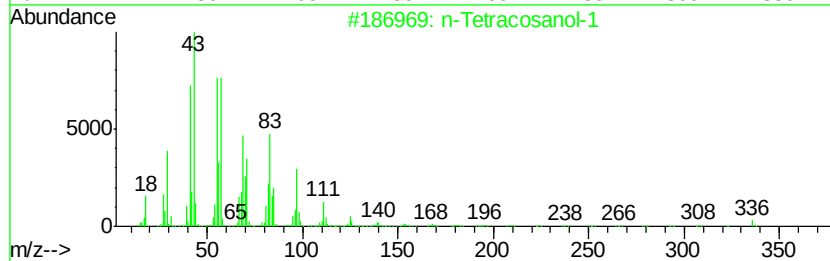
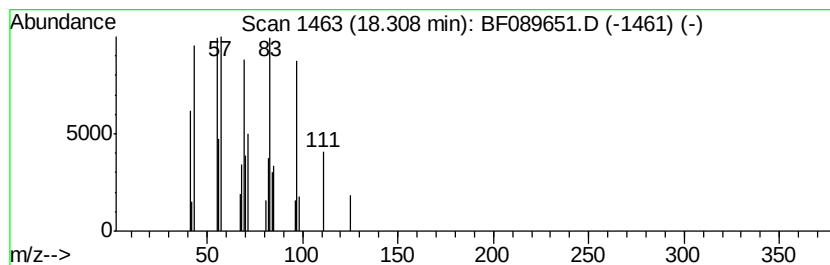
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	3.50 ng	37540	Chrysene-d12	18.39

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Tetracosanol-1	354	C24H50O	000506-51-4	80
2		1-Hexacosanol	382	C26H54O	000506-52-5	59
3		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	43
4		2,4,6,8-Tetramethyl-1-undecene	210	C15H30	059920-26-2	43
5		Cycloheptane, methyl-	112	C8H16	004126-78-7	38



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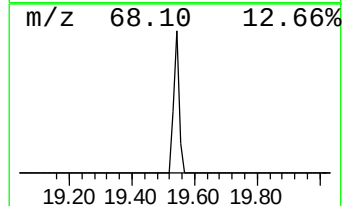
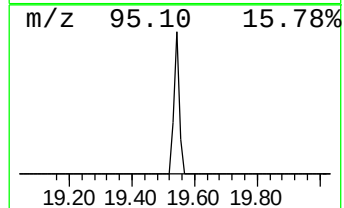
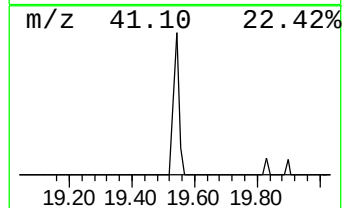
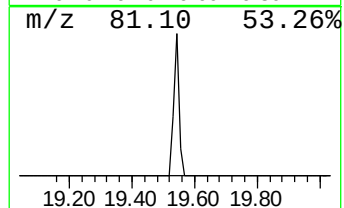
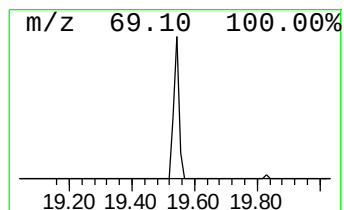
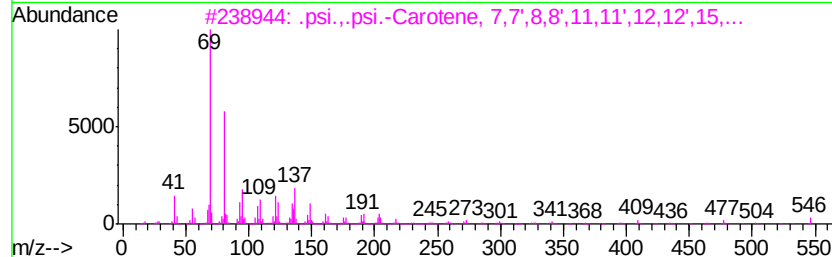
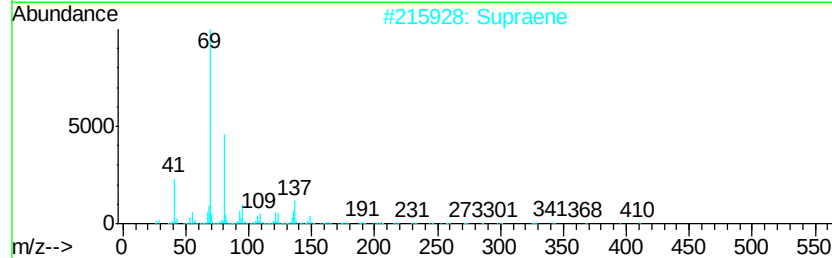
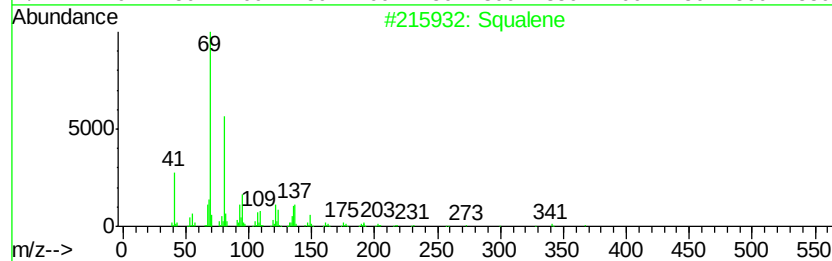
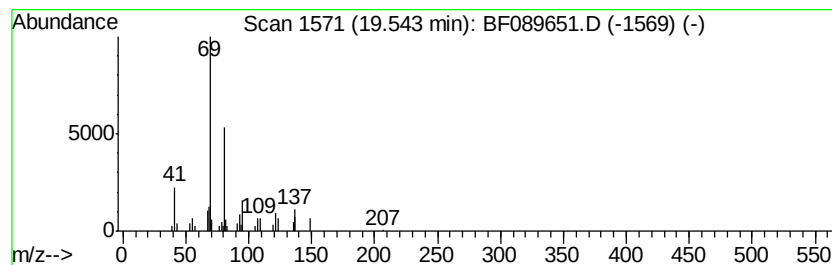
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Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.54	4.56 ng	44731	Perylene-d12	20.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	74
4	Farnesol isomer a	222	C15H26O	1000108-92-4	64
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.66	27.0	ng	296050	1	7.44	219535	20.0
unknown7.10	7.10	122.5	ng	1345050	1	7.44	219535	20.0
Hexadecane	13.92	3.1	ng	34406	4	14.69	222728	20.0
n-Tetracosanol-1	18.31	3.5	ng	37540	5	18.39	214763	20.0
Squalene	19.54	4.6	ng	44731	6	20.05	196392	20.0