

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072516\
 Data File : BF089298.D
 Acq On : 26 Jul 2016 2:48
 Operator : UM/SJ
 Sample : H4184-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-COMP

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-BF072016.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	1.701	9	10	49	rVB	1090651	2329987	100.00%	23.171%
2	4.673	268	270	277	rVB	31177	46700	2.00%	0.464%
3	5.141	309	311	331	rBV	512477	797558	34.23%	7.931%
4	6.216	403	405	413	rBV	728441	843988	36.22%	8.393%
5	6.330	413	415	433	rVB	812630	937511	40.24%	9.323%
6	6.559	433	435	446	rBV	217718	267728	11.49%	2.662%
7	6.719	446	449	451	rBV	538285	635008	27.25%	6.315%
8	7.130	483	485	500	rBV	455486	551678	23.68%	5.486%
9	7.850	545	548	550	rBV	250205	315330	13.53%	3.136%
10	8.925	640	642	658	rBV	973893	924990	39.70%	9.199%
11	9.325	675	677	679	rBV	212085	179023	7.68%	1.780%
12	9.588	698	700	703	rBV	393489	363019	15.58%	3.610%
13	10.376	767	769	779	rBV	398355	442458	18.99%	4.400%
14	11.062	827	829	843	rBV	319306	312883	13.43%	3.111%
15	12.639	965	967	970	rBV	552221	547120	23.48%	5.441%
16	13.554	1045	1047	1056	rBB	20019	36538	1.57%	0.363%
17	13.679	1056	1058	1067	rBV	257851	265830	11.41%	2.644%
18	14.537	1130	1133	1134	rBV	27071	36929	1.58%	0.367%
19	15.017	1173	1175	1182	rBV	179304	221541	9.51%	2.203%

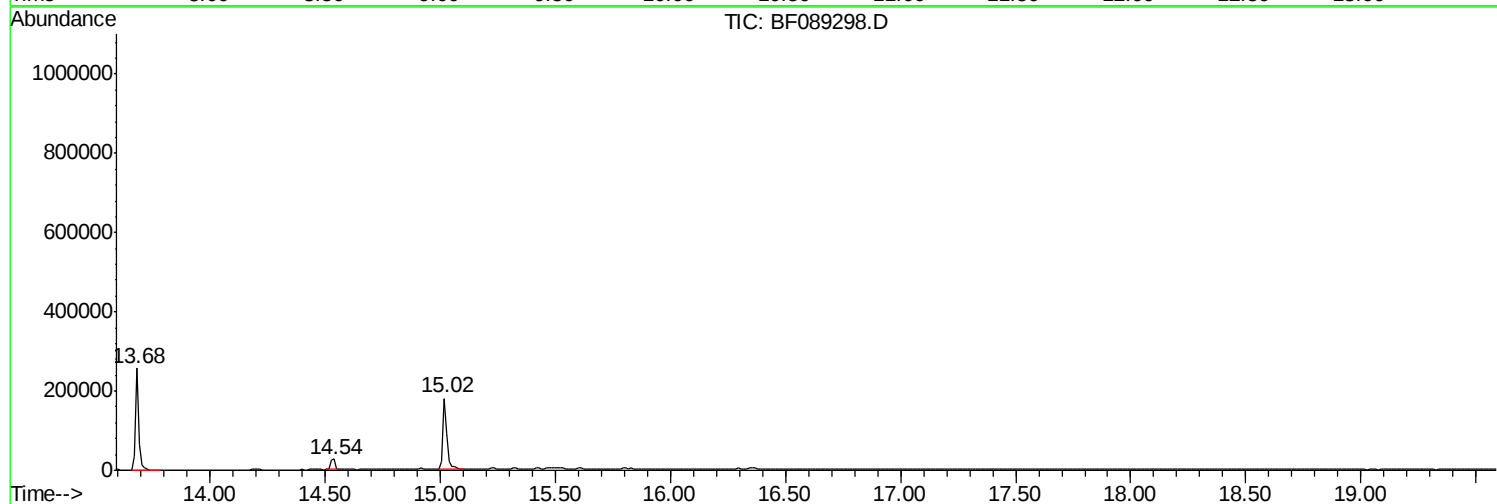
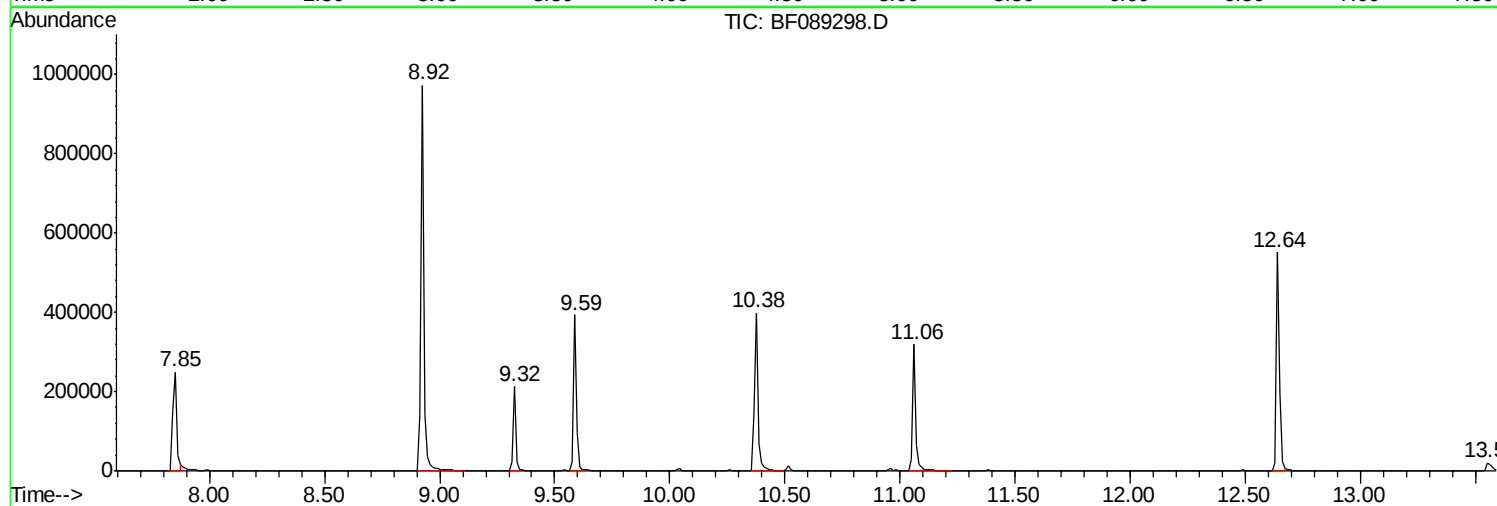
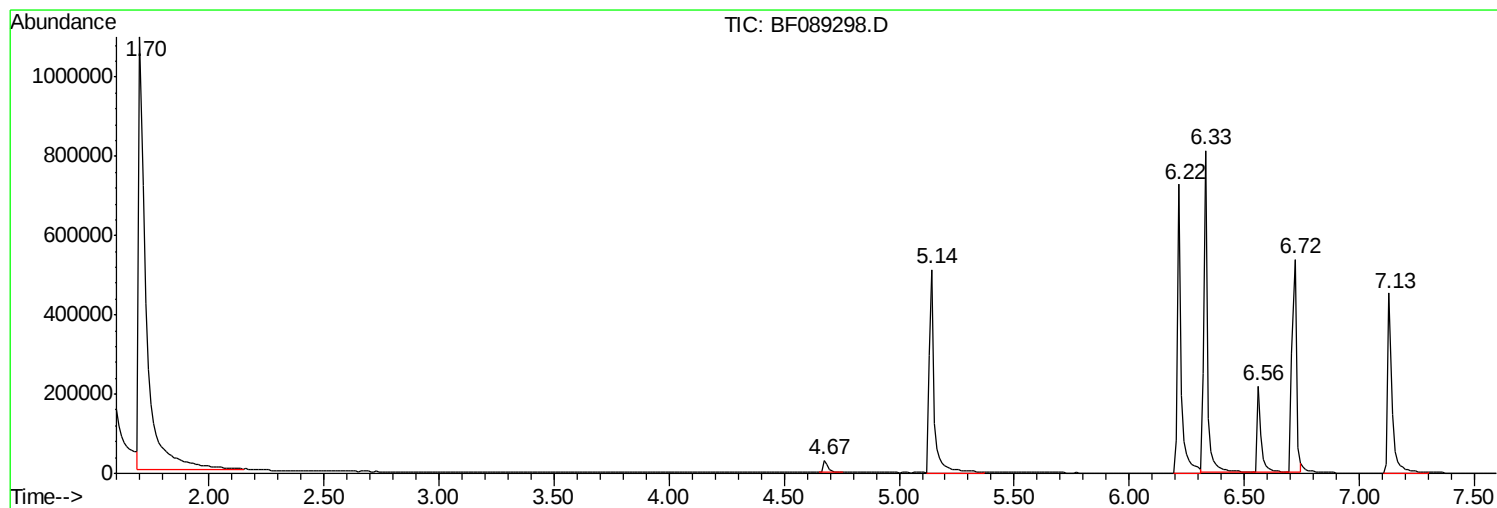
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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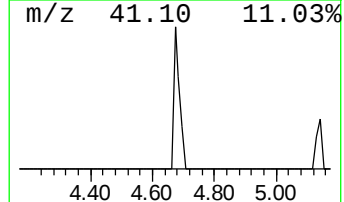
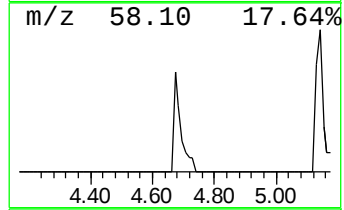
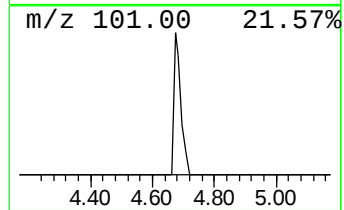
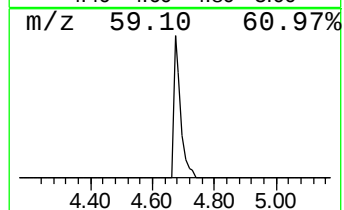
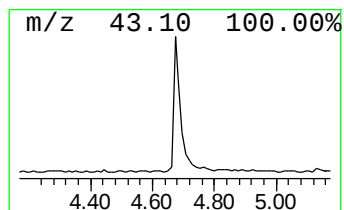
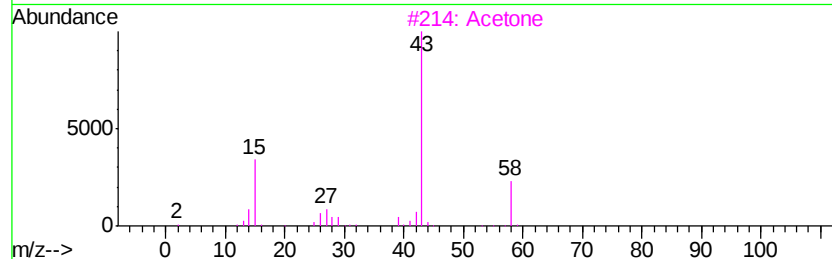
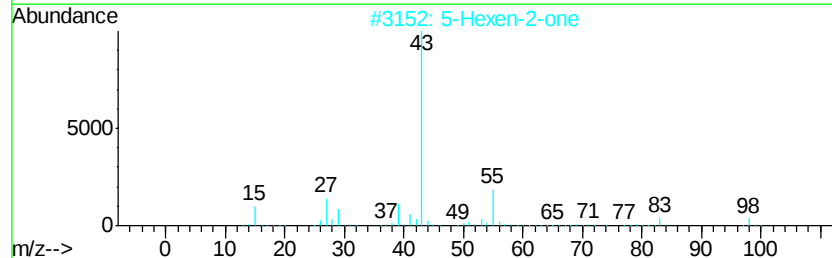
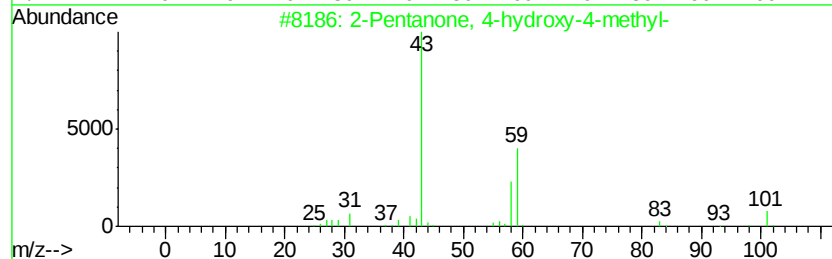
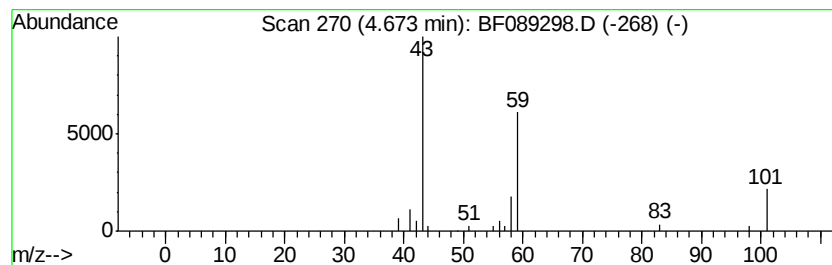
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	3.49 ng	46700	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Acetone	58	C3H6O	000067-64-1	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		Guanidine	59	CH5N3	000113-00-8	5



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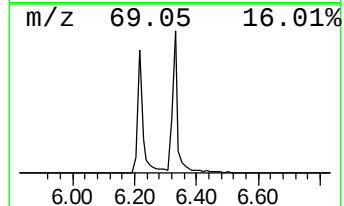
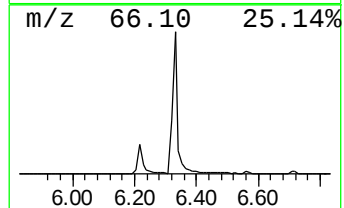
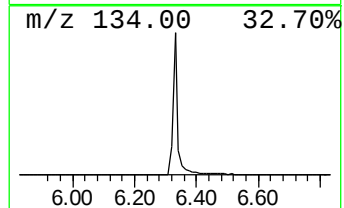
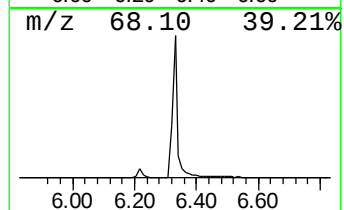
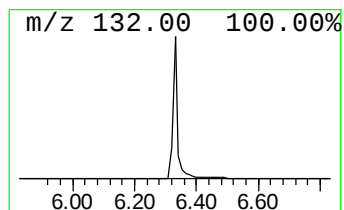
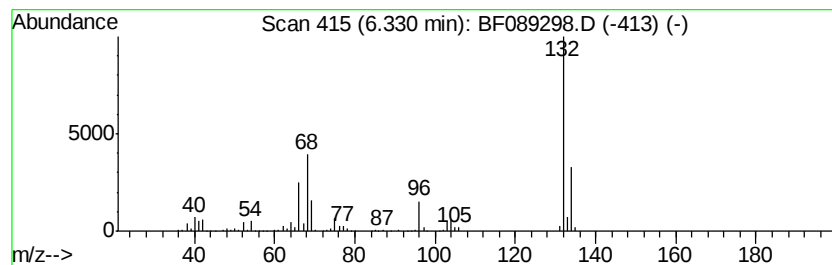
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Peak Number 3 unknown6.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	70.03 ng	937511	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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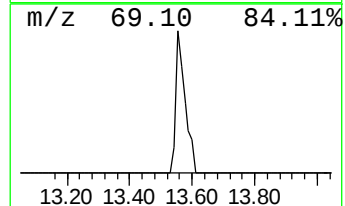
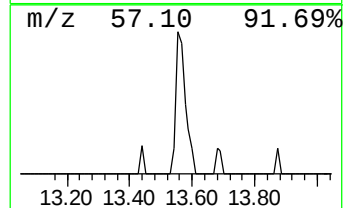
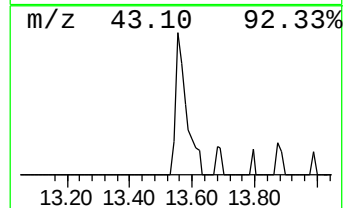
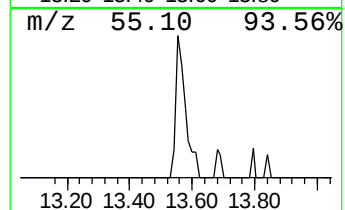
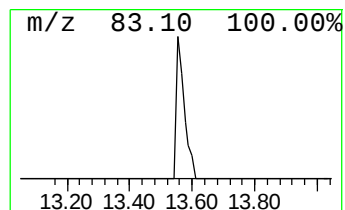
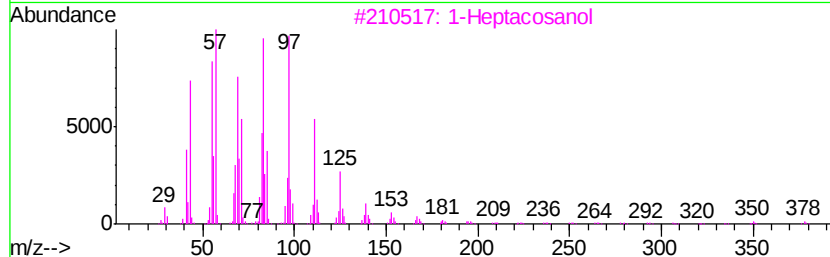
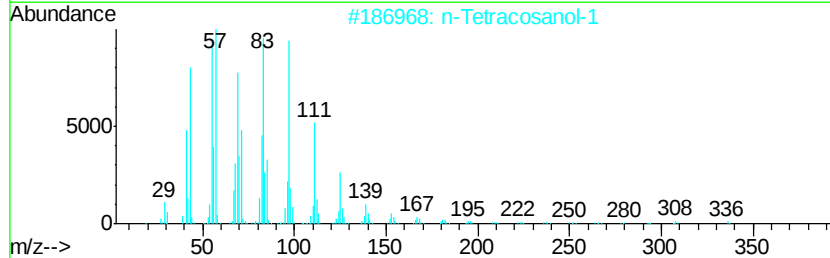
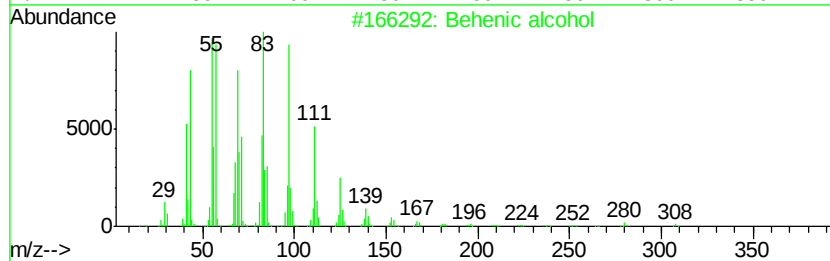
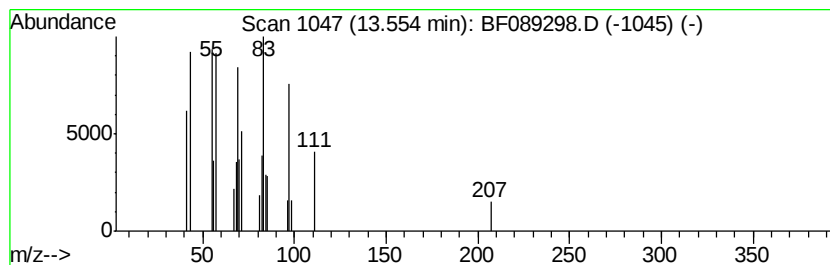
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Peak Number 5 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	2.75 ng	36538	Chrysene-d12	13.68

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	91
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



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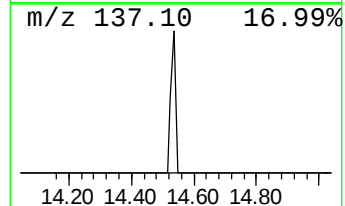
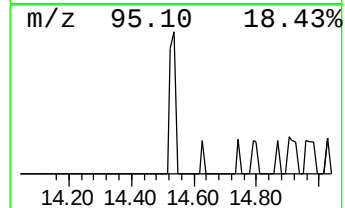
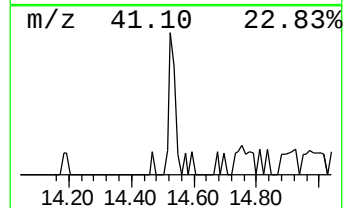
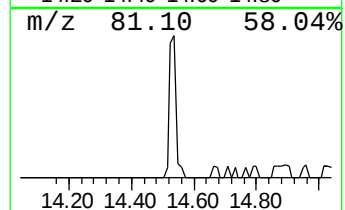
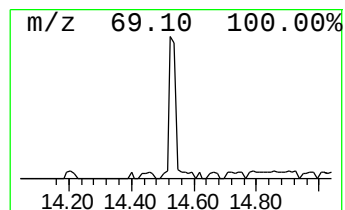
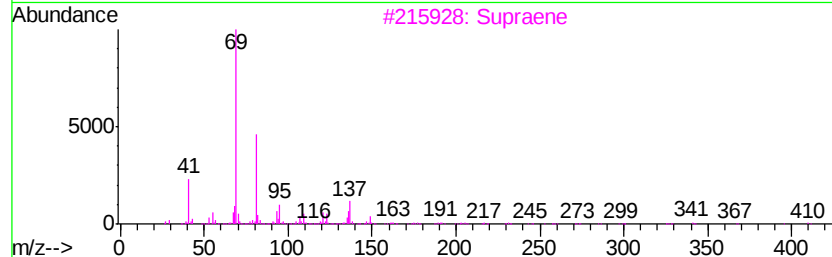
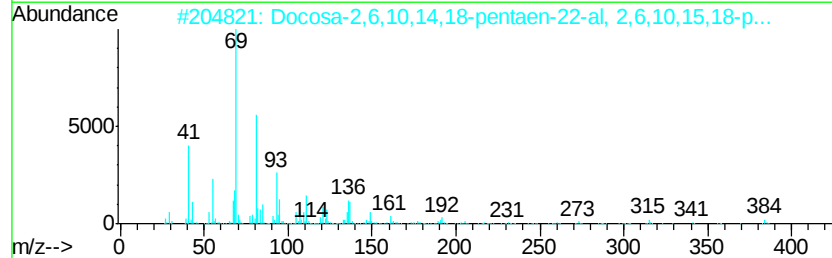
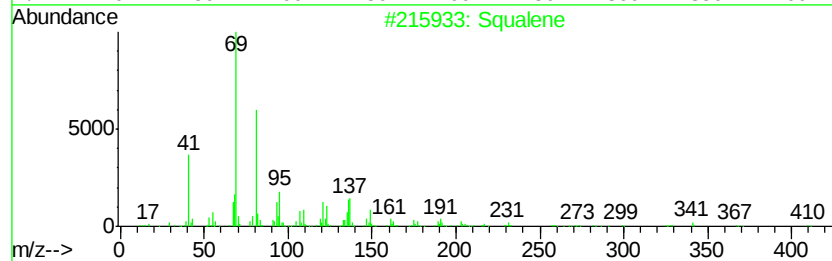
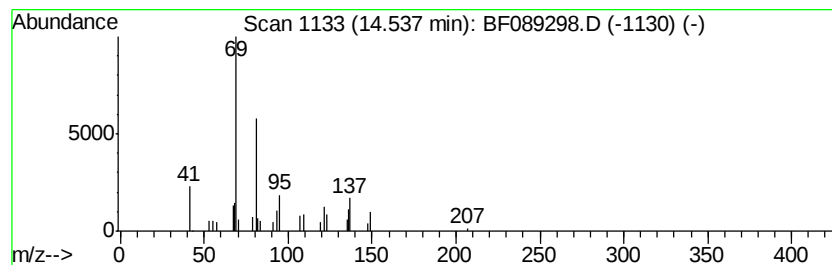
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	3.33 ng	36929	Perylene-d12	15.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
3		Supraene	410	C30H50	007683-64-9	78
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	78
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.67	3.5	ng	46700	1	6.56	267728	20.0
unknown6.33	6.33	70.0	ng	937511	1	6.56	267728	20.0
Behenic alcohol	13.55	2.8	ng	36538	5	13.68	265830	20.0
Squalene	14.54	3.3	ng	36929	6	15.02	221541	20.0