

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052016\
 Data File : BF087256.D
 Acq On : 21 May 2016 7:12
 Operator : UM/SJ
 Sample : H3167-04
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RAV-RMW-3

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-BF051716.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	8	10	21	rVB	419001	727417	13.69%	2.103%
2	4.673	269	270	287	rBV	430586	738635	13.90%	2.136%
3	5.141	309	311	330	rBV	1420564	2019540	38.01%	5.839%
4	6.216	404	405	413	rBV	746237	1339411	25.21%	3.873%
5	6.330	413	415	417	rBV	2610196	3410536	64.20%	9.861%
6	6.559	433	435	440	rBV	587933	878842	16.54%	2.541%
7	6.707	446	448	451	rBV	3432426	3109959	58.54%	8.992%
8	6.833	455	459	463	rVB2	23040	59394	1.12%	0.172%
9	7.130	482	485	494	rBV	2617340	2846281	53.58%	8.229%
10	7.839	545	547	550	rBV	1058477	1137967	21.42%	3.290%
11	8.925	639	642	644	rBV	4810401	5312612	100.00%	15.360%
12	9.325	675	677	681	rBV	150253	154497	2.91%	0.447%
13	9.530	693	695	697	rBV	64558	68127	1.28%	0.197%
14	9.588	697	700	703	rBV	1464759	1358516	25.57%	3.928%
15	10.033	736	739	740	rBV	111596	102127	1.92%	0.295%
16	10.250	755	758	761	rBV	31742	55329	1.04%	0.160%
17	10.376	766	769	772	rBV	2613937	2758684	51.93%	7.976%
18	10.502	777	780	787	rVB	117800	165608	3.12%	0.479%
19	10.948	816	819	823	rVB2	45264	53432	1.01%	0.154%
20	11.062	827	829	832	rBV	1415004	1302988	24.53%	3.767%
21	11.611	875	877	888	rBV2	41145	79141	1.49%	0.229%
22	12.651	965	968	970	rBV	4722067	4685680	88.20%	13.548%
23	13.611	1048	1052	1057	rBV	53535	201065	3.78%	0.581%
24	13.691	1057	1059	1065	rVB	1073036	1099160	20.69%	3.178%
25	14.525	1129	1132	1134	rBV	175982	163618	3.08%	0.473%
26	15.040	1175	1177	1189	rVB	592874	758415	14.28%	2.193%

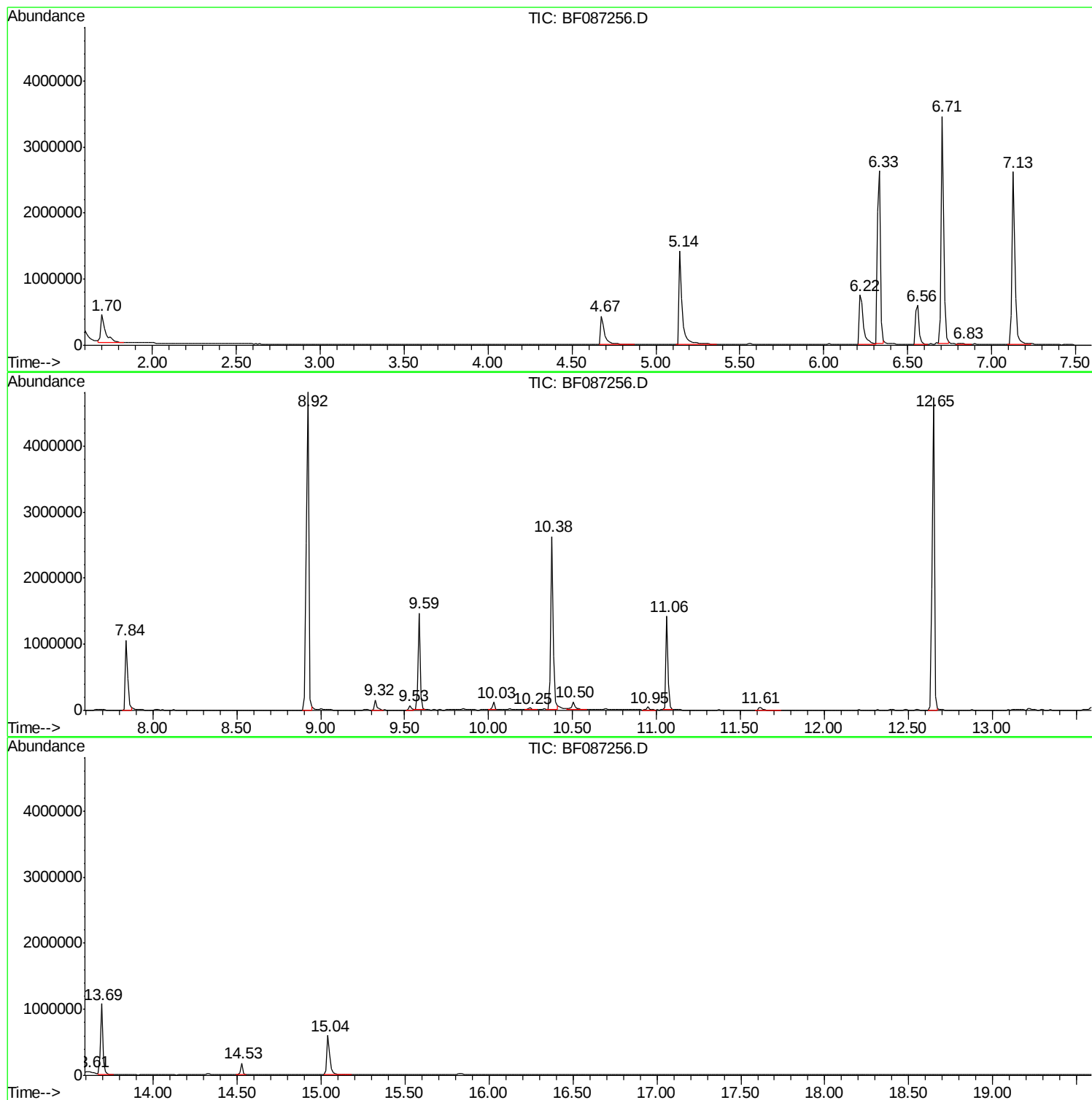
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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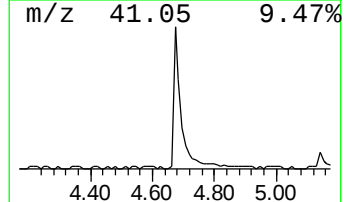
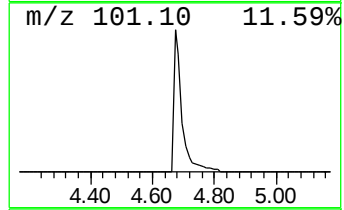
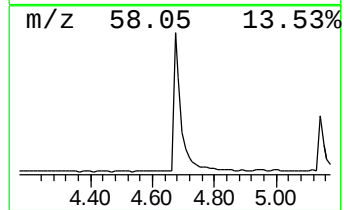
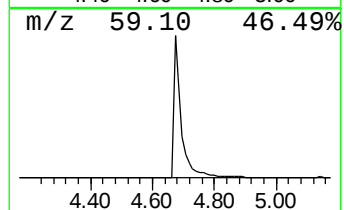
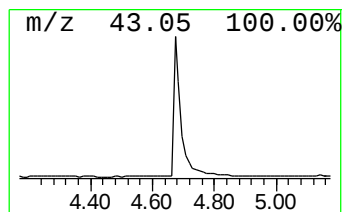
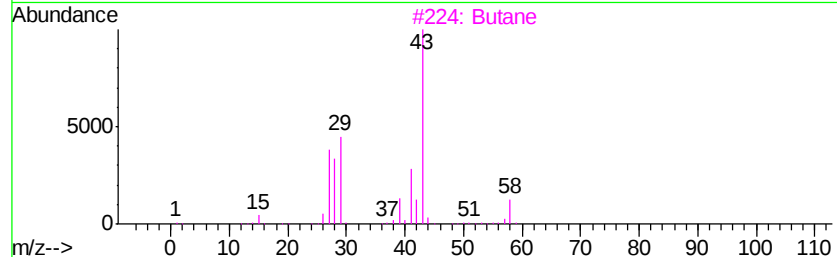
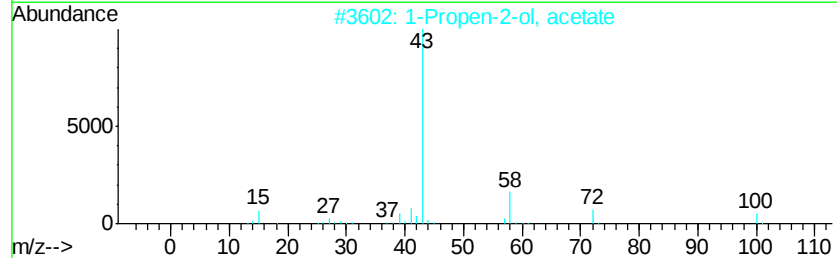
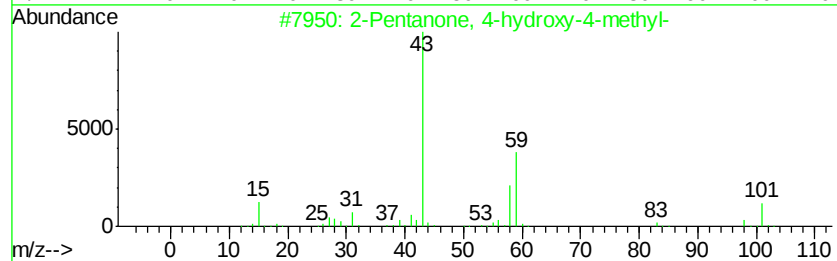
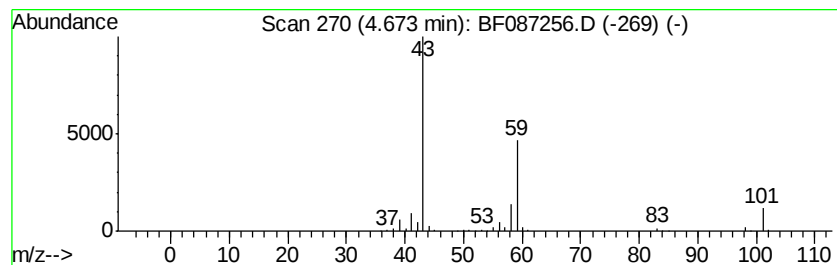
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF051716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	16.81 ng	738635	1,4-Dichlorobenzene-d4	6.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		Butane	58	C4H10	000106-97-8	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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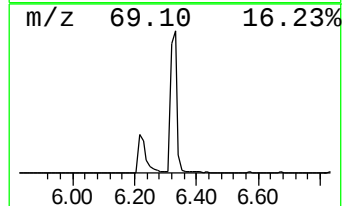
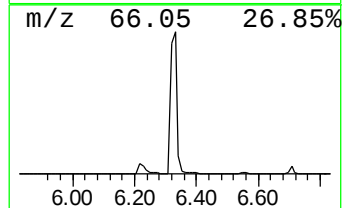
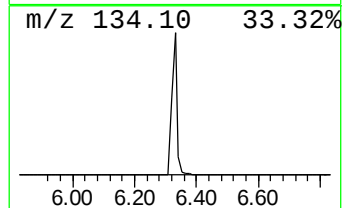
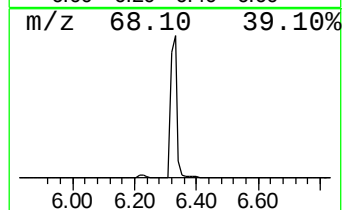
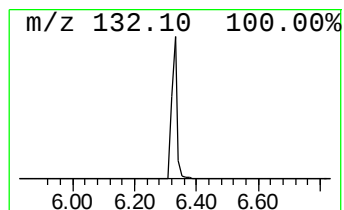
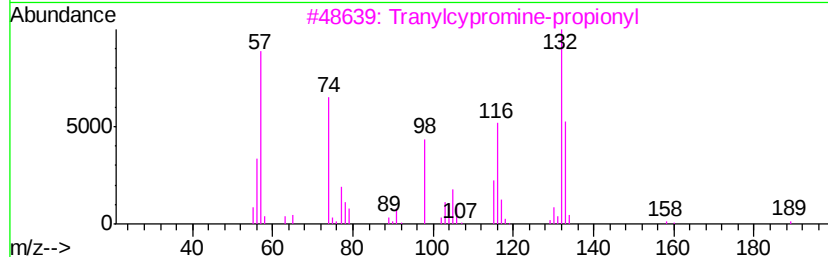
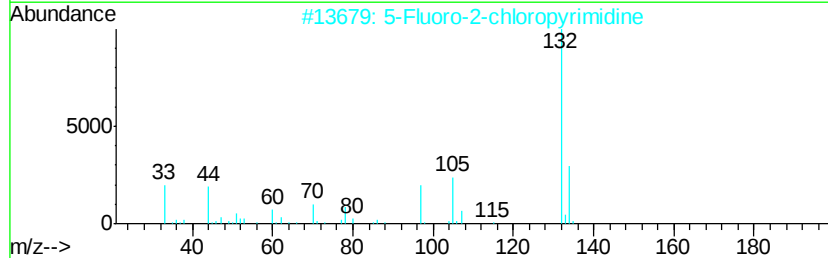
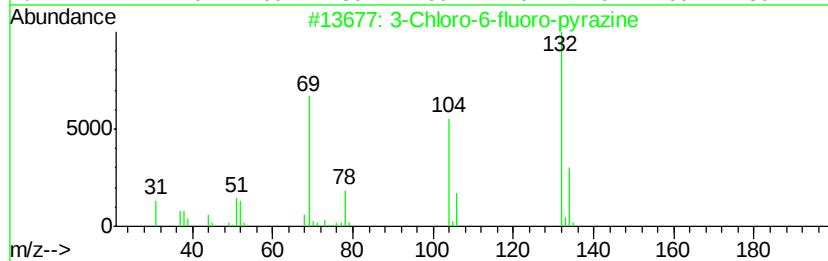
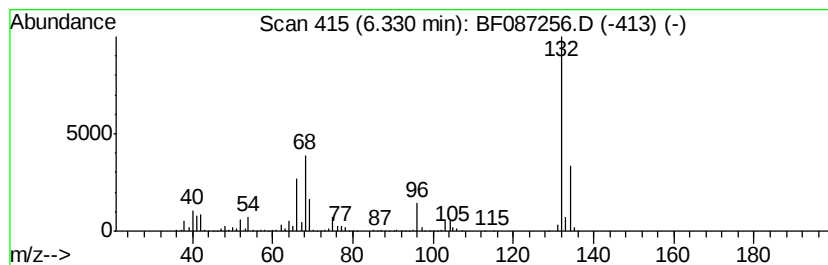
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Peak Number 3 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	77.61 ng	3410540	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		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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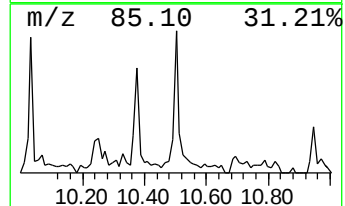
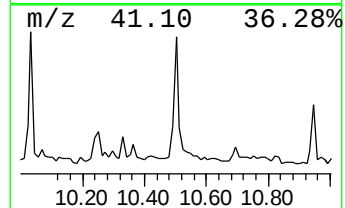
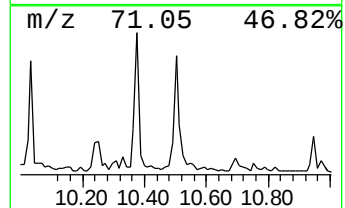
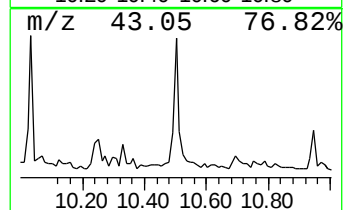
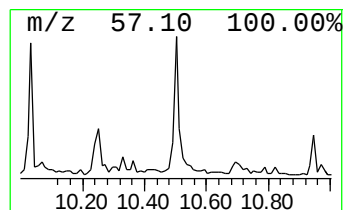
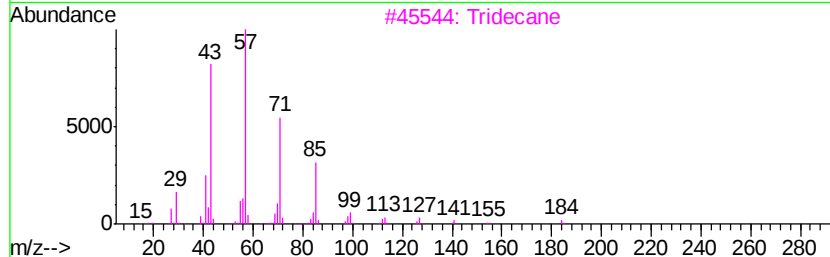
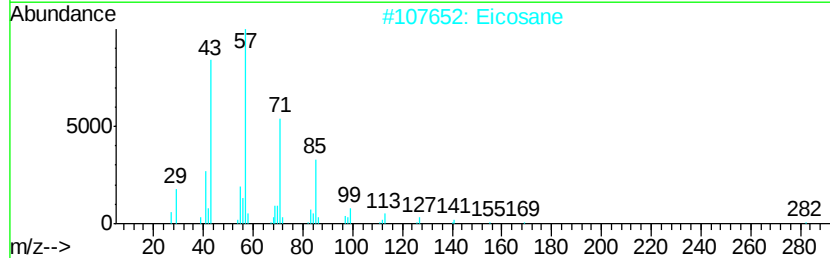
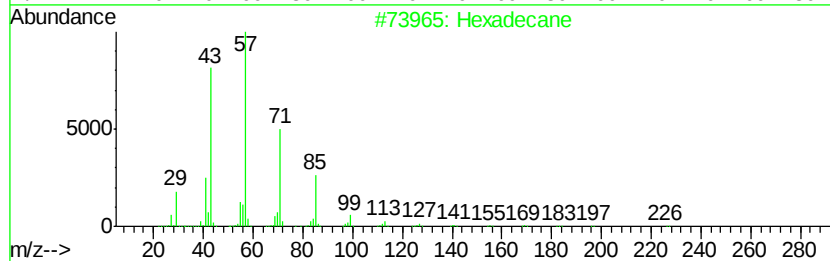
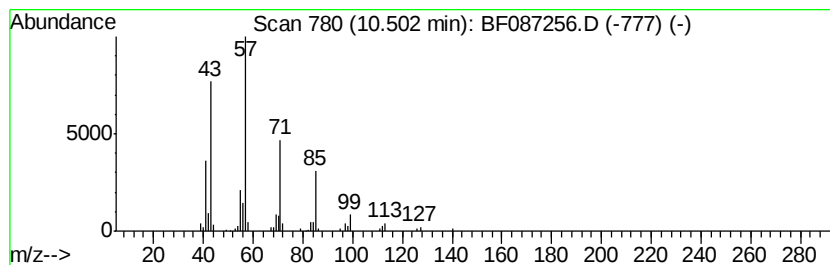
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.50	2.54 ng	165608	Phenanthrene-d10		11.06
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Eicosane	282	C20H42	000112-95-8	91
3	Tridecane	184	C13H28	000629-50-5	86
4	Nonadecane	268	C19H40	000629-92-5	72
5	Heptadecane, 2,6-dimethyl-	268	C19H40	054105-67-8	72



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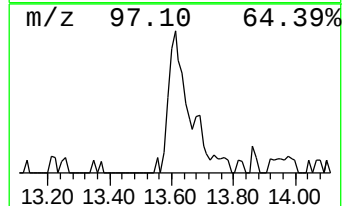
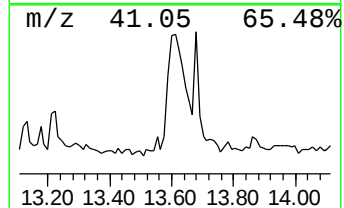
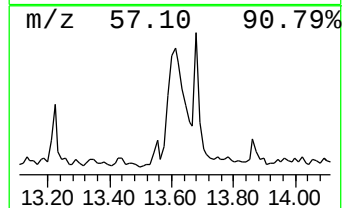
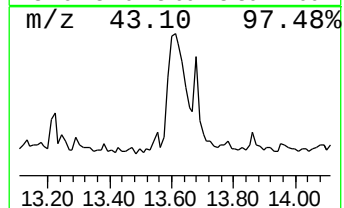
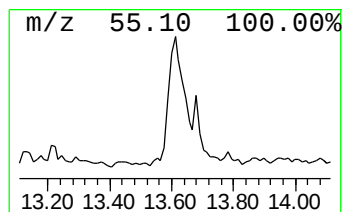
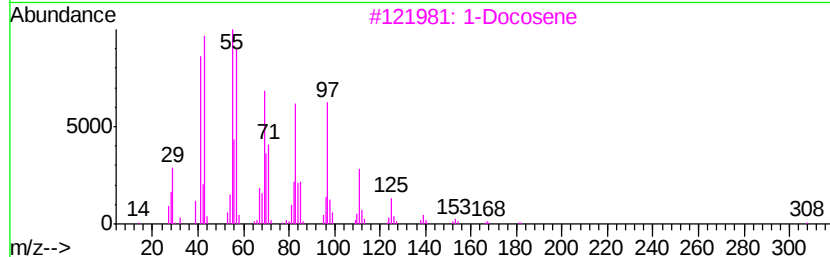
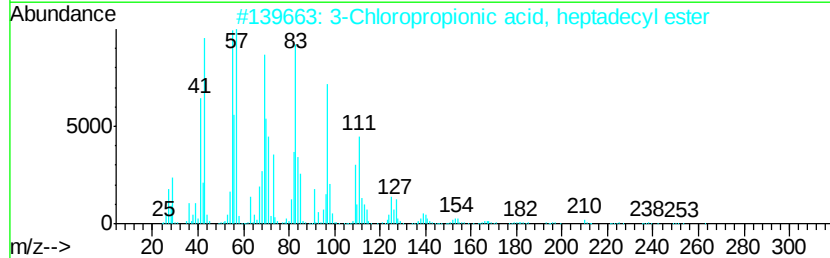
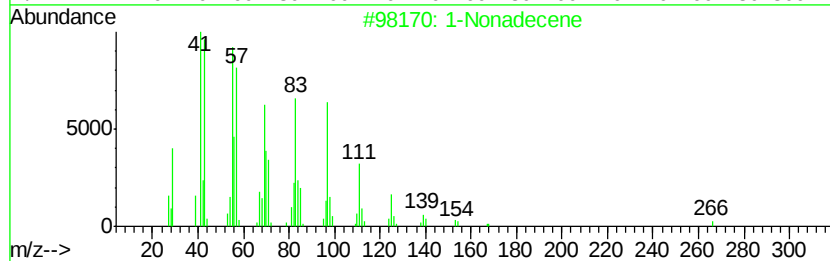
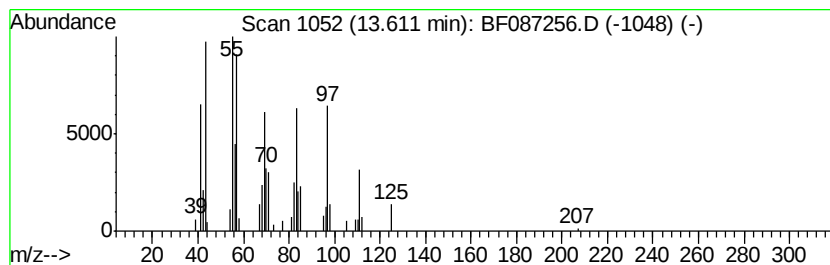
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Peak Number 6 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.61	3.66 ng	201065	Chrysene-d12	13.69	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	91
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
3	1-Docosene	308	C22H44	001599-67-3	91
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5	Hexadecen-1-ol, trans-9-	240	C16H32O	064437-47-4	90



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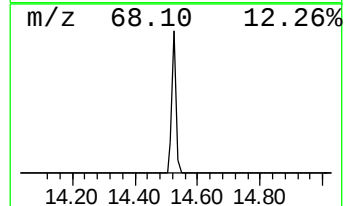
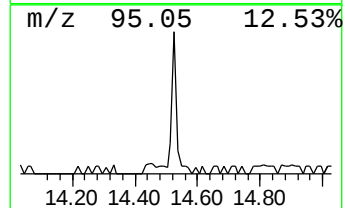
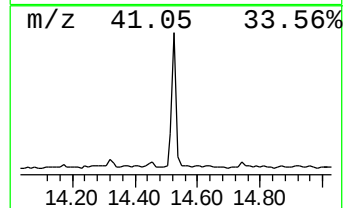
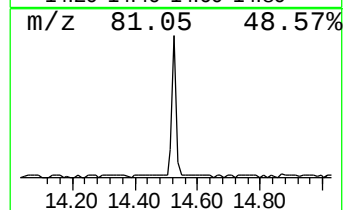
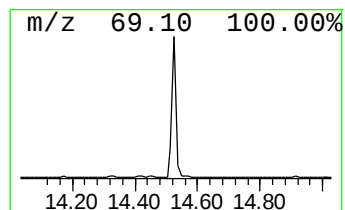
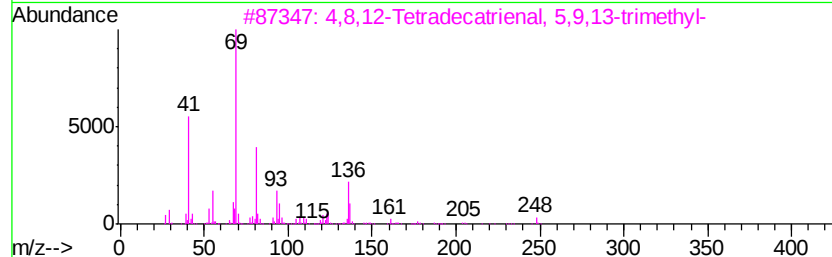
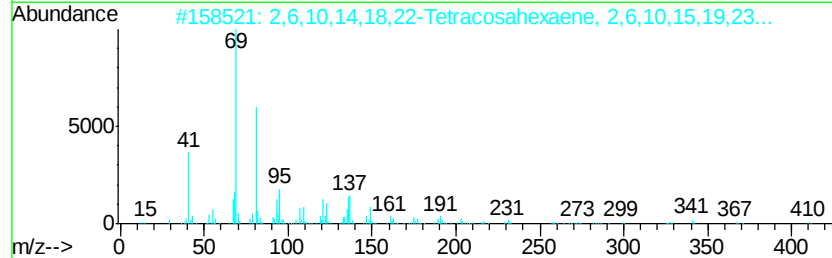
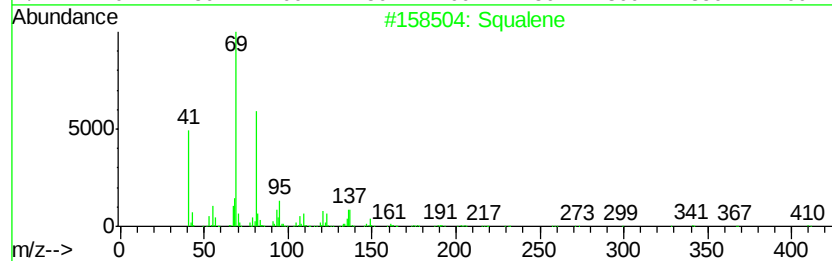
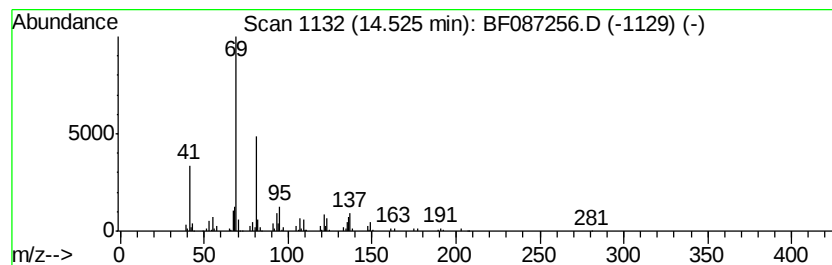
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Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	4.31 ng	163618	Perylene-d12	15.04
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	80
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203 C12H17N3	003974-79-6	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.67	16.8	ng	738635	1	6.56	878842	20.0
unknown6.33	6.33	77.6	ng	3410540	1	6.56	878842	20.0
Hexadecane	10.50	2.5	ng	165608	4	11.06	1302990	20.0
1-Nonadecene	13.61	3.7	ng	201065	5	13.69	1099160	20.0
Squalene	14.53	4.3	ng	163618	6	15.04	758415	20.0