

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111217\
 Data File : BF100494.D
 Acq On : 12 Nov 2017 17:13
 Operator : SJ/JU
 Sample : I6403-07
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110817-TIDO-F-U-B

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-BF110817.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	2.204	16	20	26	rVB	75070	108796	3.63%	0.554%
2	5.116	512	515	525	rBV	199242	194392	6.48%	0.990%
3	5.510	578	582	586	rBV	996859	923868	30.79%	4.703%
4	6.510	749	752	756	rBV2	637040	633227	21.10%	3.223%
5	6.545	756	758	762	rVB	37872	32749	1.09%	0.167%
6	6.663	774	778	782	rBV	1734553	1638706	54.61%	8.341%
7	6.898	815	818	822	rBV	978768	840536	28.01%	4.279%
8	7.057	841	845	848	rBV	2546368	2244882	74.81%	11.427%
9	7.463	909	914	917	rBV	1924881	1764157	58.79%	8.980%
10	8.181	1032	1036	1040	rBV	1263975	1034305	34.47%	5.265%
11	9.257	1214	1219	1222	rBV	3347348	3000753	100.00%	15.275%
12	9.645	1282	1285	1299	rBV	218828	182282	6.07%	0.928%
13	9.886	1323	1326	1329	rBV	100300	83603	2.79%	0.426%
14	9.939	1329	1335	1347	rVB	1088321	1022432	34.07%	5.204%
15	10.645	1451	1455	1461	rBV	55680	46033	1.53%	0.234%
16	10.722	1464	1468	1479	rBV	1025088	878857	29.29%	4.474%
17	11.422	1583	1587	1591	rBV	947549	800731	26.68%	4.076%
18	11.639	1621	1624	1634	rBV	48214	59127	1.97%	0.301%
19	12.192	1715	1718	1721	rVB	90772	66886	2.23%	0.340%
20	12.757	1810	1814	1822	rBV	45100	40873	1.36%	0.208%
21	12.821	1822	1825	1828	rVB	118104	85887	2.86%	0.437%
22	13.010	1852	1857	1860	rBV	2193867	2124743	70.81%	10.816%
23	13.527	1941	1945	1948	rBV	73789	59771	1.99%	0.304%
24	14.063	2032	2036	2044	rVB	872100	761285	25.37%	3.875%
25	14.910	2176	2180	2184	rBV	288635	283325	9.44%	1.442%
26	15.174	2221	2225	2231	rVB	27237	31924	1.06%	0.163%
27	15.545	2283	2288	2299	rBV	400450	567501	18.91%	2.889%
28	16.009	2361	2367	2372	rBV	30302	45361	1.51%	0.231%
29	16.527	2450	2455	2462	rVB2	31100	55391	1.85%	0.282%
30	17.133	2553	2558	2565	rVB2	17246	32845	1.09%	0.167%

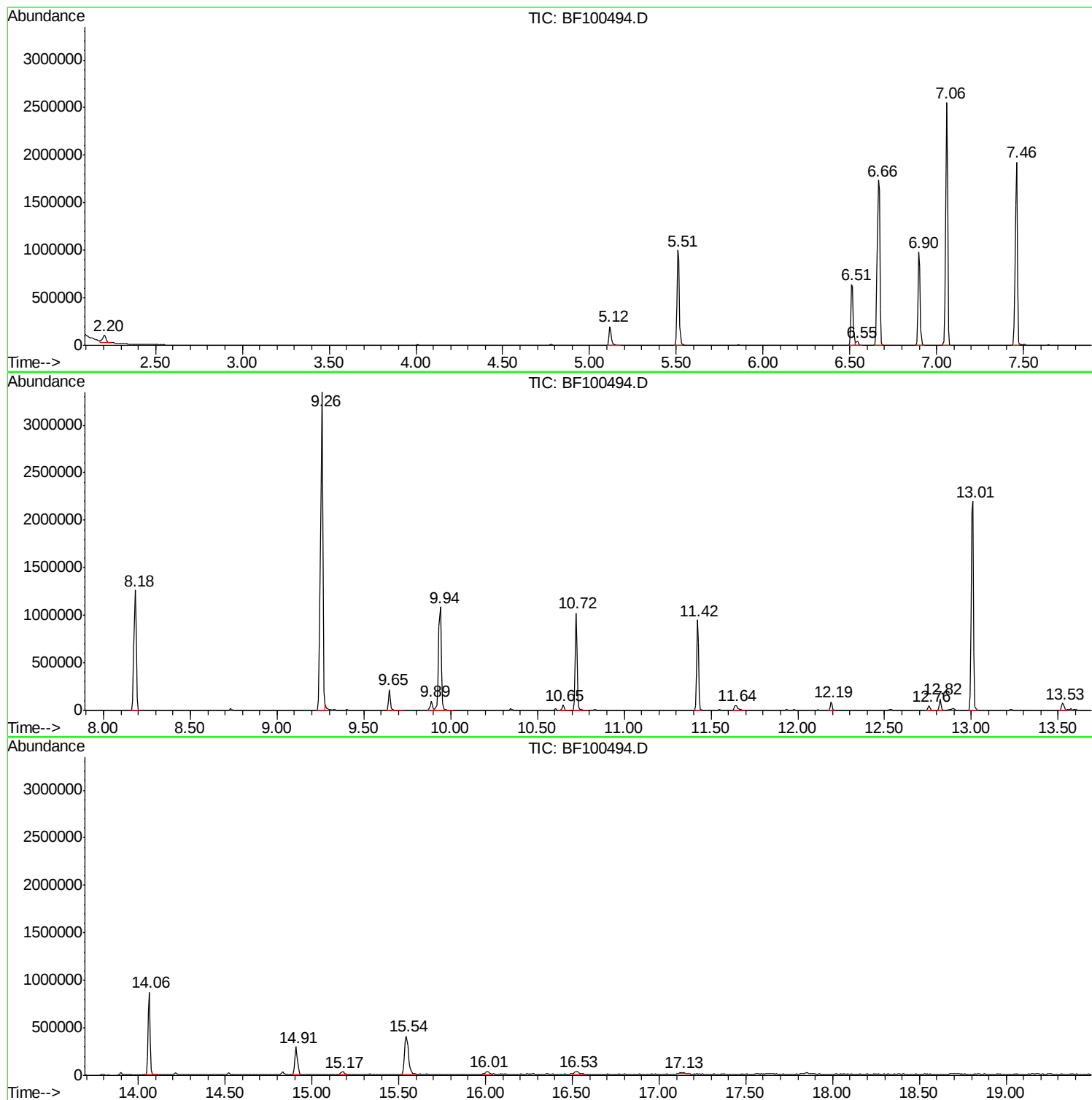
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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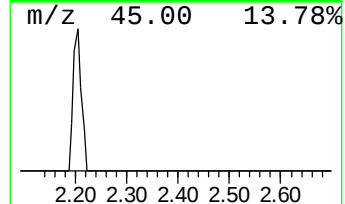
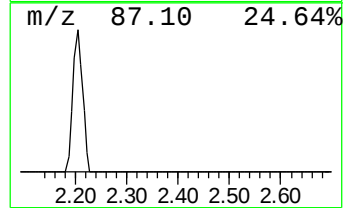
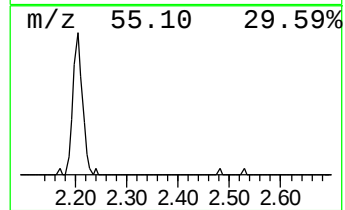
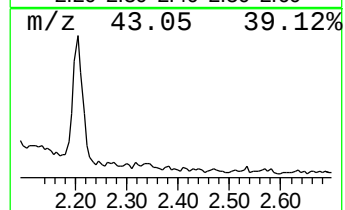
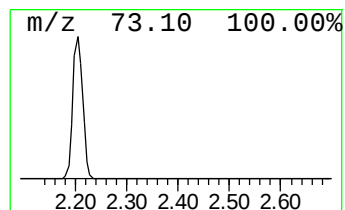
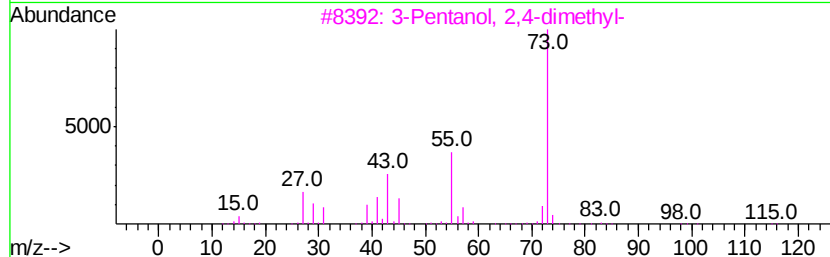
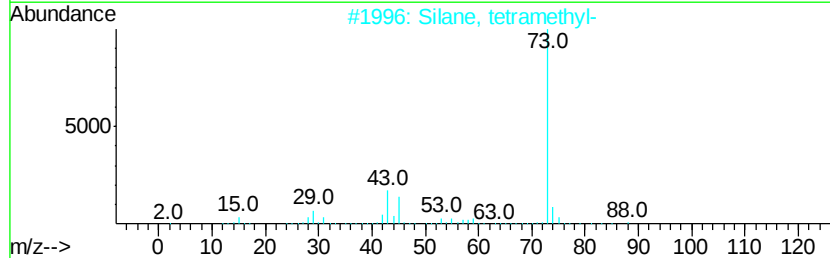
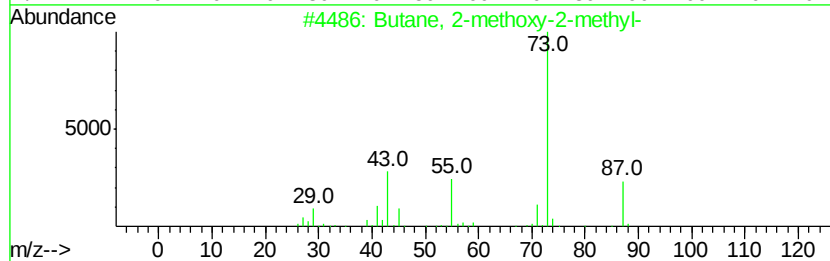
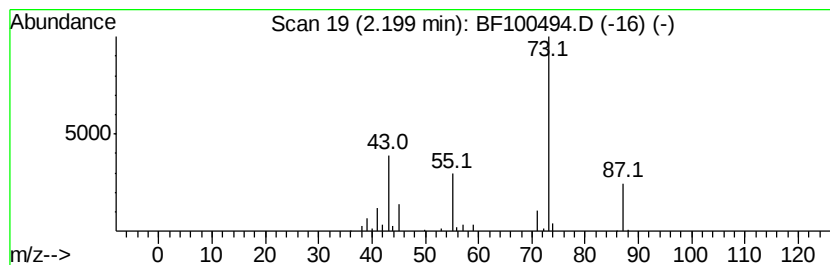
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.59 ng	108796	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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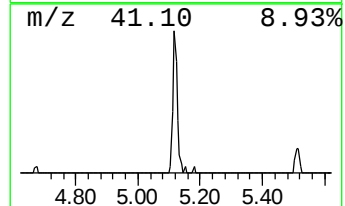
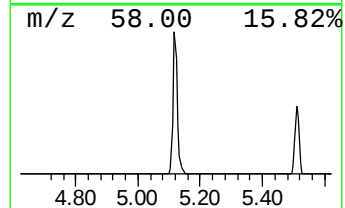
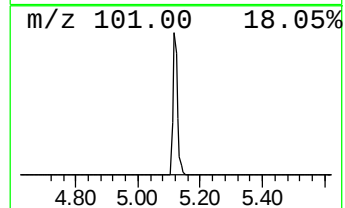
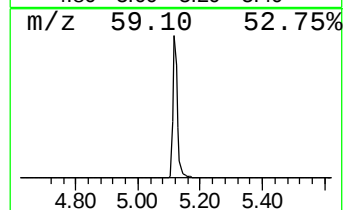
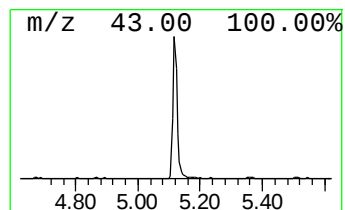
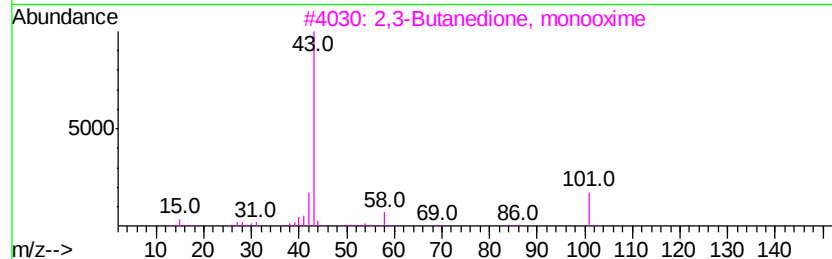
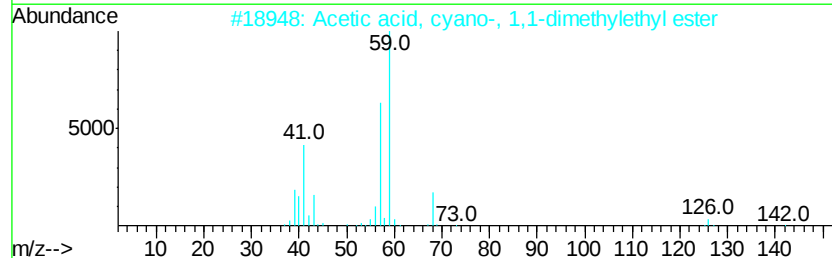
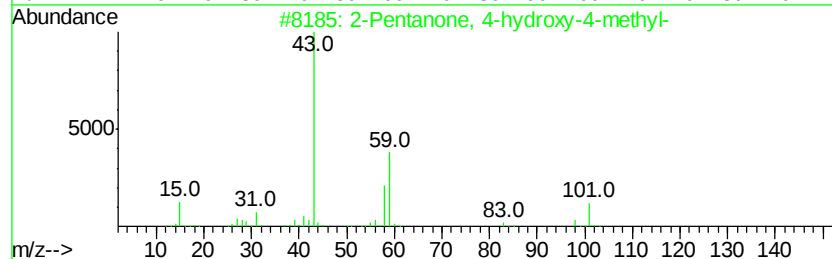
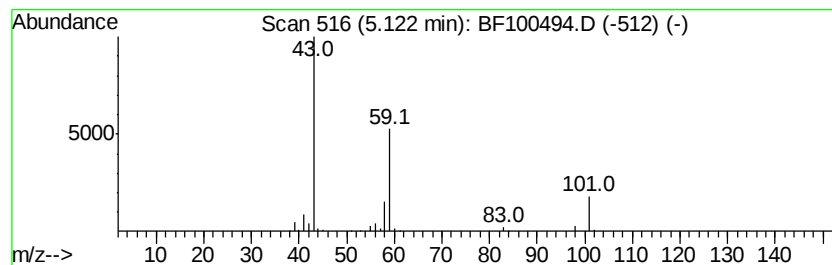
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.63 ng	194392	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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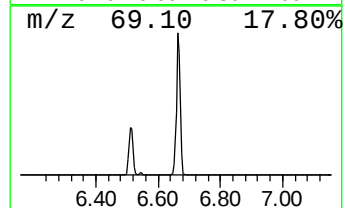
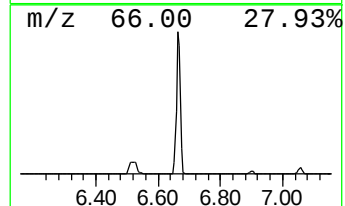
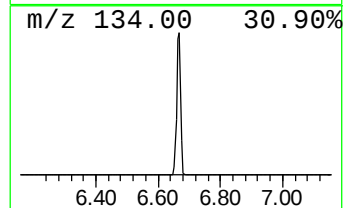
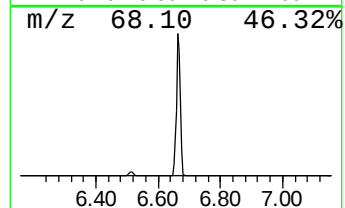
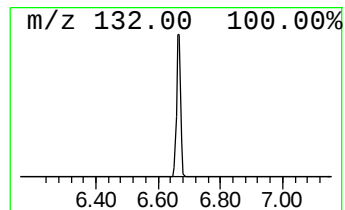
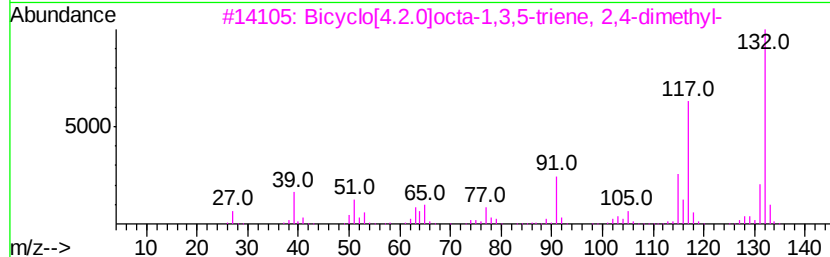
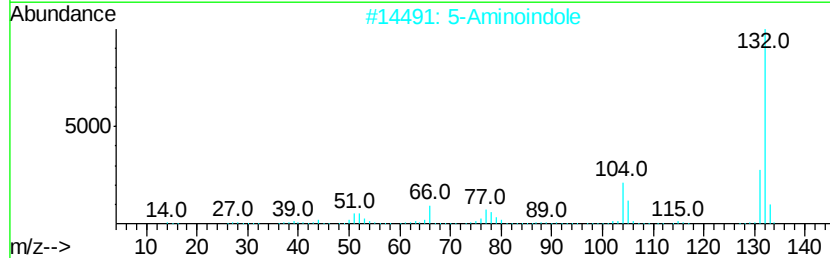
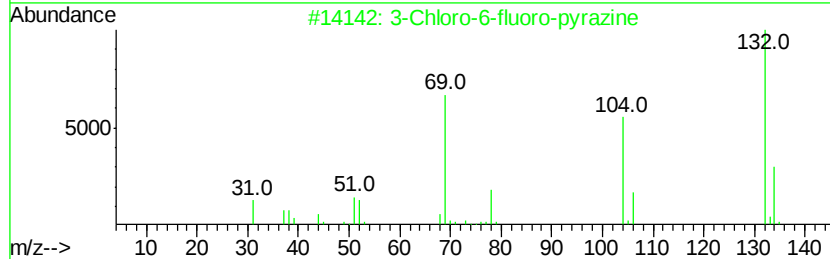
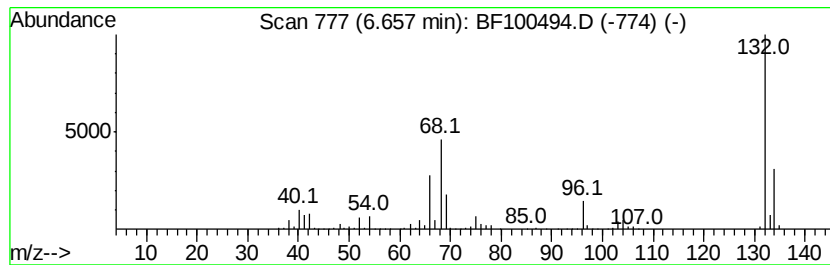
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Peak Number 3 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	38.99 ng	1638710	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Bicyclo[4.2.0]octa-1,3,5-triene, ...	132	C10H12	028749-81-7	9	
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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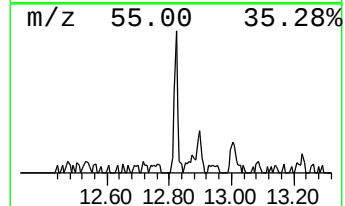
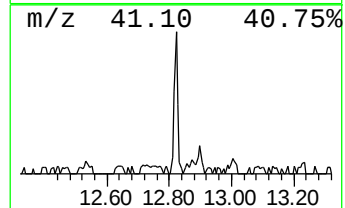
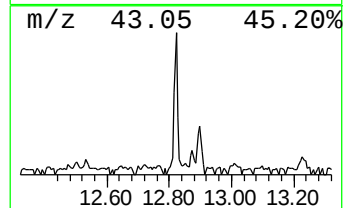
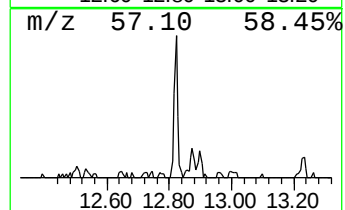
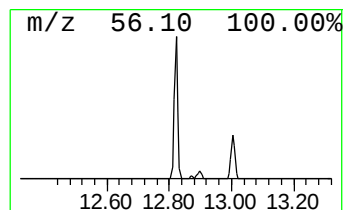
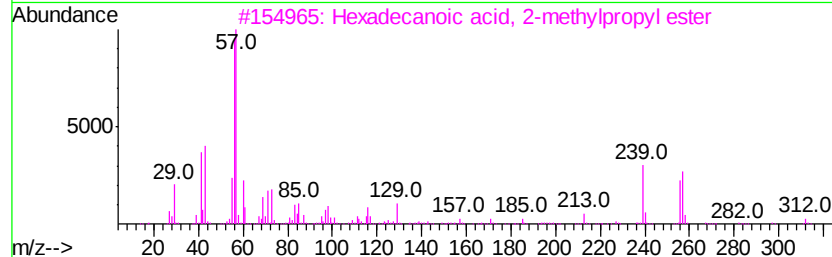
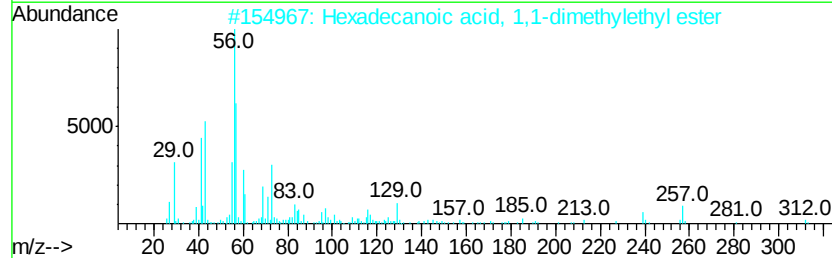
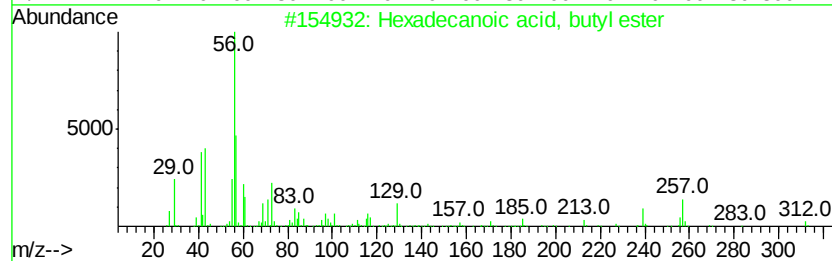
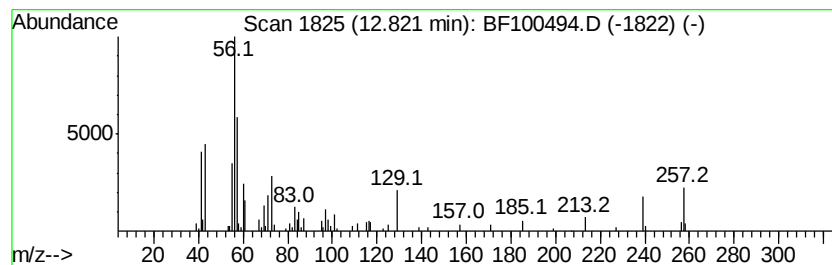
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.82	2.26 ng	85887	Chrysene-d12	14.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	87
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	72
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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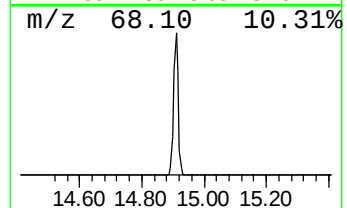
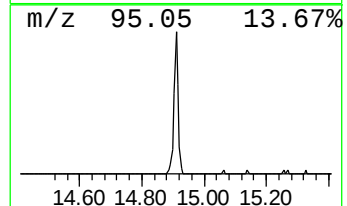
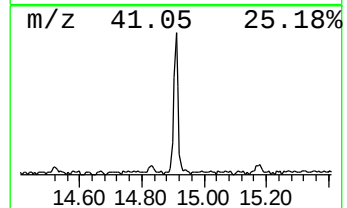
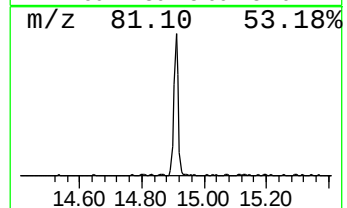
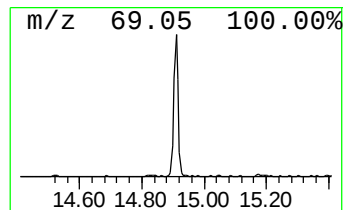
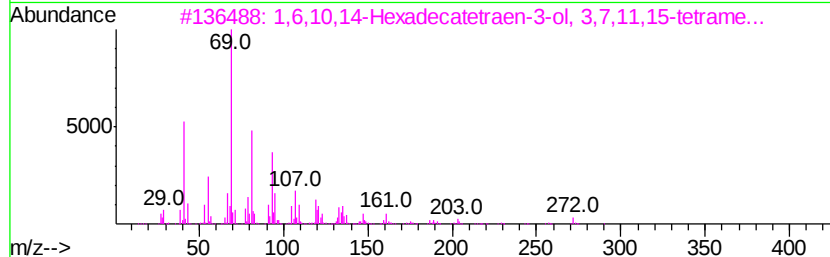
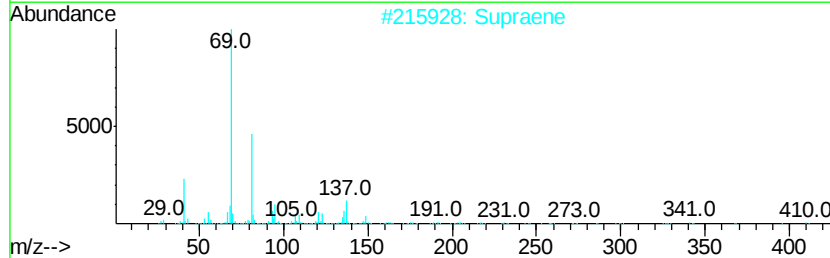
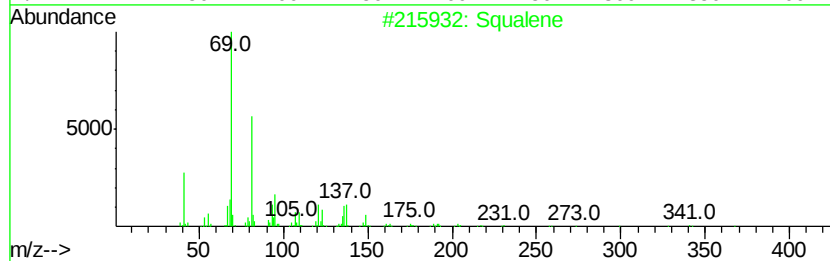
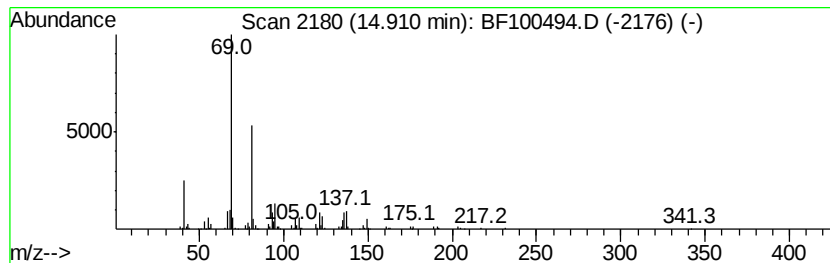
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Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	9.99 ng	283325	Perylene-d12	15.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	59
4		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50
5		Methanone, dicyclopropyl-	110	C7H10O	001121-37-5	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	2.6	ng	108796	1	6.90	840536	20.0
2-Pentanone, 4-hy...	5.12	4.6	ng	194392	1	6.90	840536	20.0
unknown6.66	6.66	39.0	ng	1638710	1	6.90	840536	20.0
Hexadecanoic acid...	12.82	2.3	ng	85887	5	14.06	761285	20.0
Squalene	14.91	10.0	ng	283325	6	15.54	567501	20.0