

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121719\
 Data File : BF118242.D
 Acq On : 17 Dec 2019 22:40
 Operator : JU
 Sample : K6324-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-11

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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	2.134	3	8	20	rVB	280945	388543	15.58%	1.788%
2	5.069	503	507	518	rVB	302885	358713	14.38%	1.651%
3	5.481	572	577	597	rBV	2180730	2067267	82.88%	9.513%
4	6.493	744	749	768	rBV	2298872	2190343	87.82%	10.080%
5	6.628	768	772	776	rBV	2632468	2355635	94.44%	10.840%
6	6.857	808	811	828	rVB	820103	680992	27.30%	3.134%
7	7.016	834	838	841	rBV	2253985	1821413	73.03%	8.382%
8	7.422	903	907	924	rBV	1379355	1329675	53.31%	6.119%
9	8.145	1026	1030	1047	rBV	927184	848664	34.03%	3.905%
10	9.222	1209	1213	1229	rBV	2642907	2494226	100.00%	11.478%
11	9.622	1277	1281	1292	rBV	97476	92734	3.72%	0.427%
12	9.910	1326	1330	1343	rBV	1046686	913964	36.64%	4.206%
13	10.698	1460	1464	1480	rBV	1444783	1359850	54.52%	6.258%
14	11.398	1580	1583	1593	rBV	792654	778477	31.21%	3.582%
15	11.922	1669	1672	1684	rBV2	76478	92279	3.70%	0.425%
16	12.992	1850	1854	1857	rBV	2210591	1978333	79.32%	9.104%
17	13.886	1999	2006	2018	rBV	160590	283327	11.36%	1.304%
18	14.051	2031	2034	2044	rVB	743936	733966	29.43%	3.378%
19	14.210	2057	2061	2064	rBV	31455	27926	1.12%	0.129%
20	14.510	2109	2112	2115	rBV	47399	56248	2.26%	0.259%
21	14.821	2162	2165	2169	rBV	55461	54568	2.19%	0.251%
22	15.168	2220	2224	2230	rBV	57169	66065	2.65%	0.304%
23	15.545	2283	2288	2297	rBV	451453	660699	26.49%	3.040%
24	15.998	2362	2365	2370	rVB2	47330	64376	2.58%	0.296%
25	16.515	2450	2453	2457	rBV5	22808	32019	1.28%	0.147%

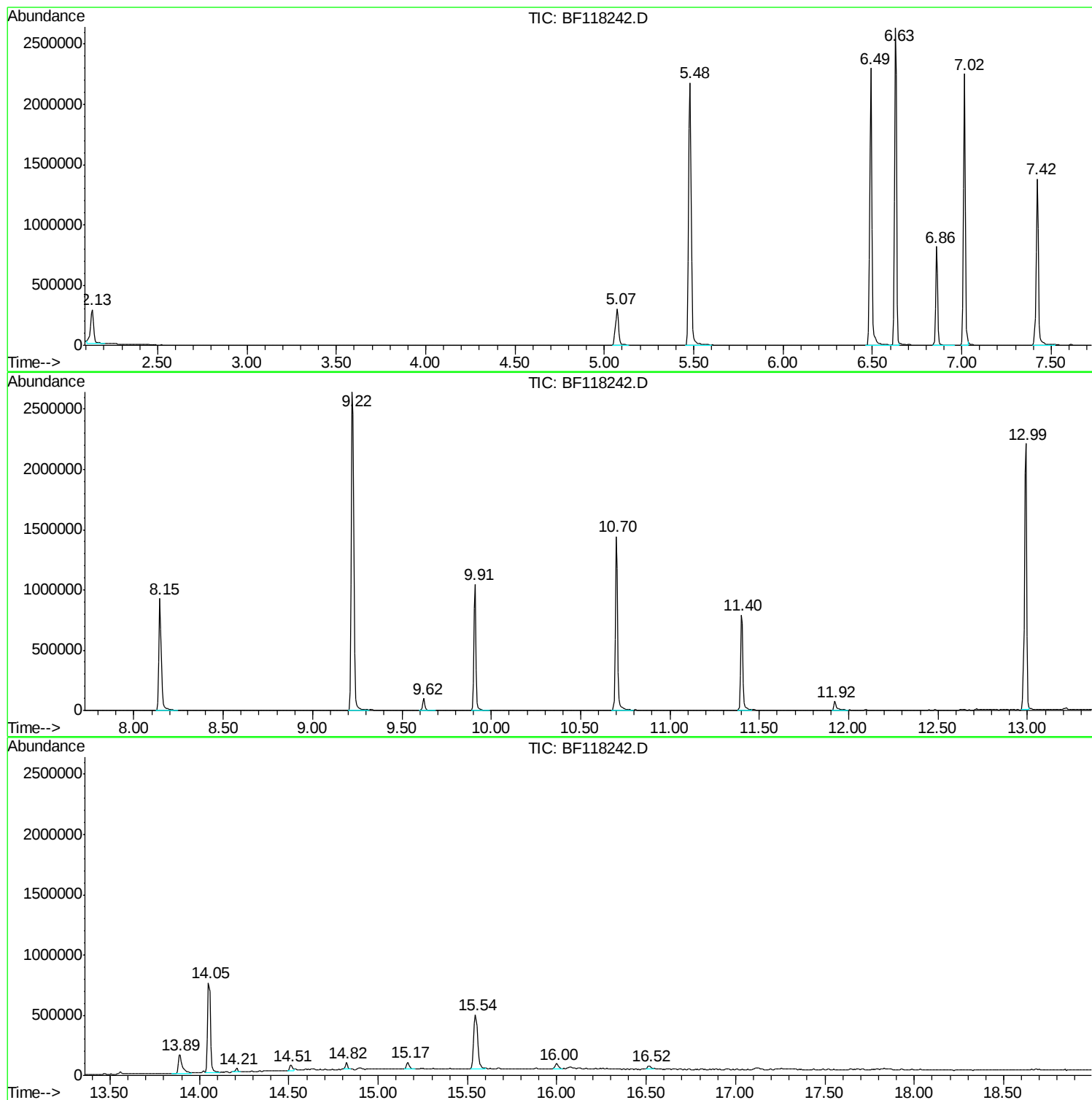
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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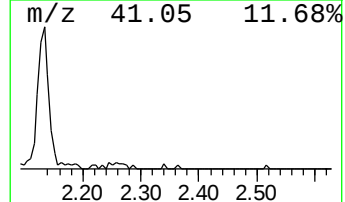
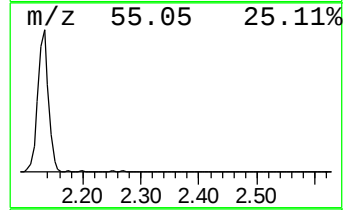
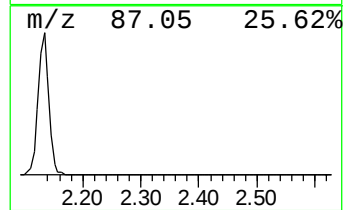
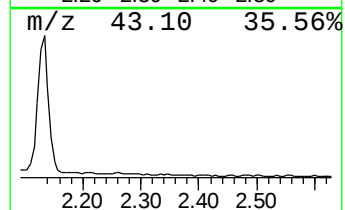
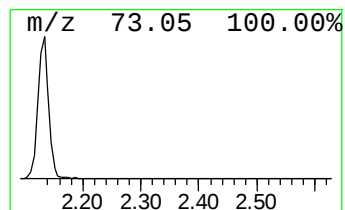
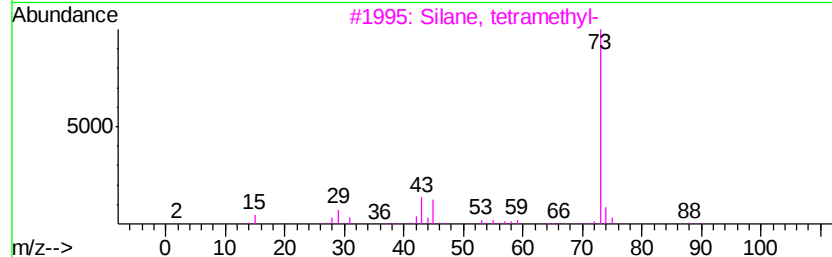
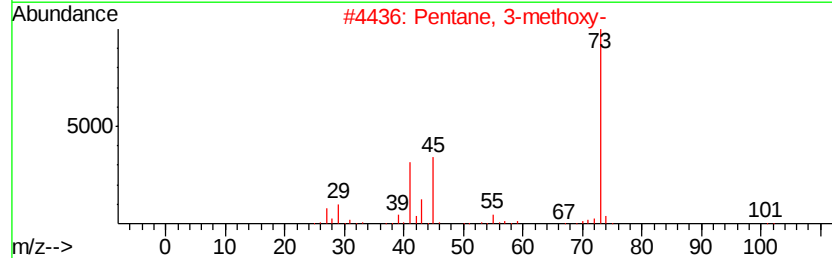
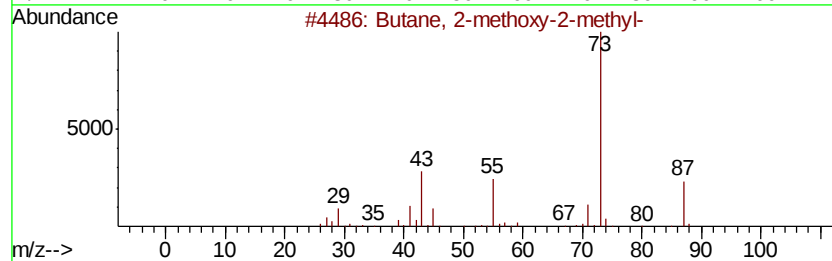
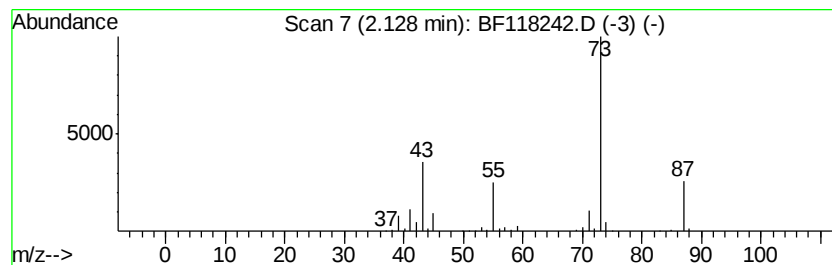
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	11.41 ng	388543	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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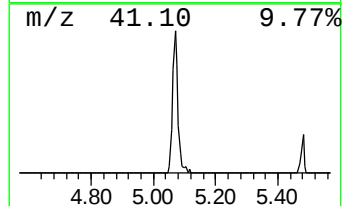
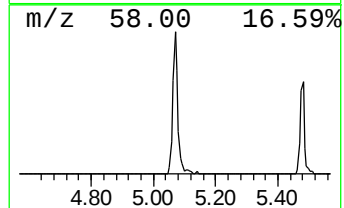
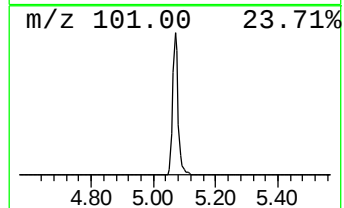
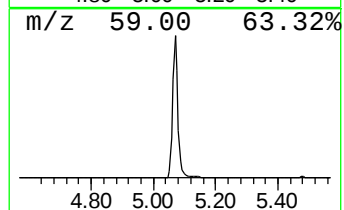
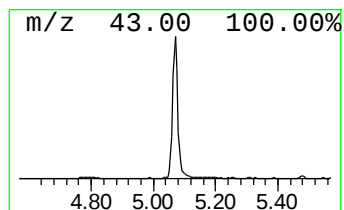
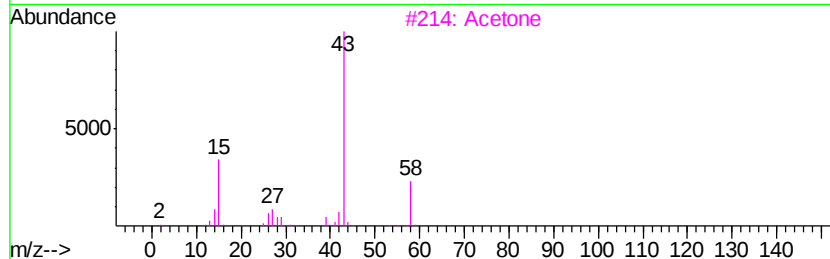
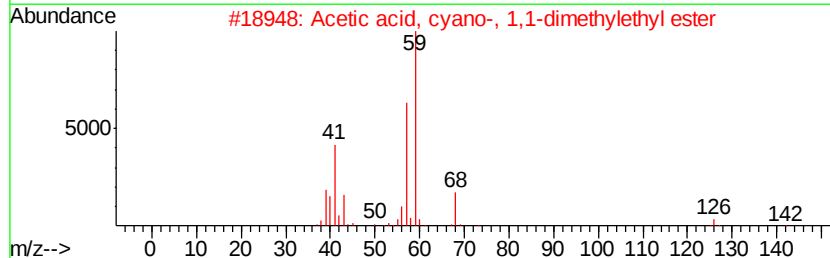
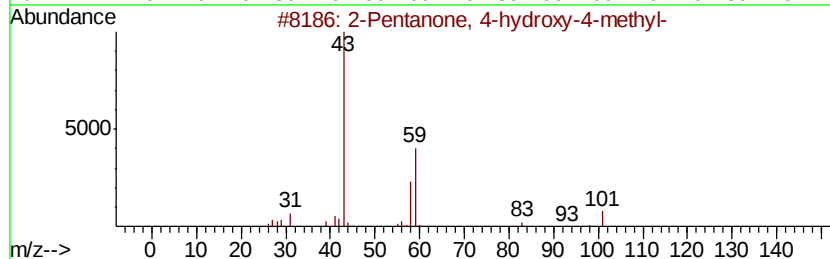
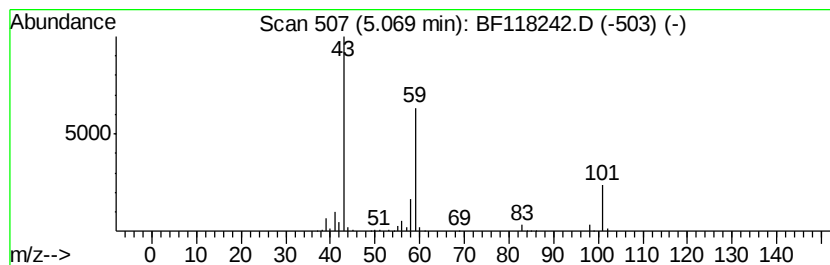
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	10.54 ng	358713	1,4-Dichlorobenzene-d4	6.86

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-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Acetone	58	C3H6O	000067-64-1	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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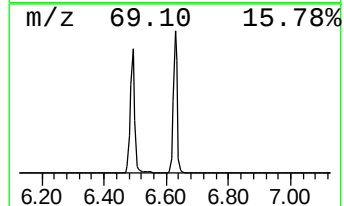
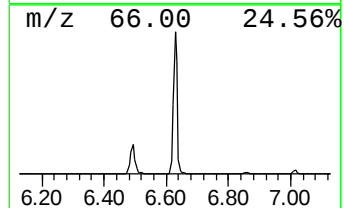
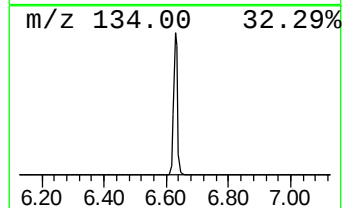
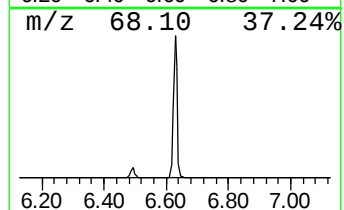
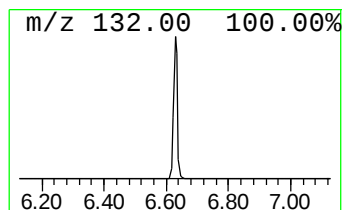
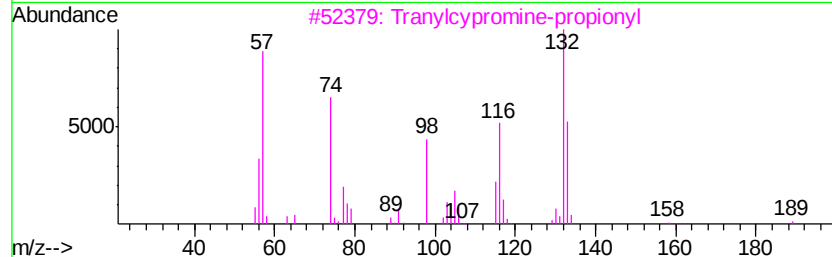
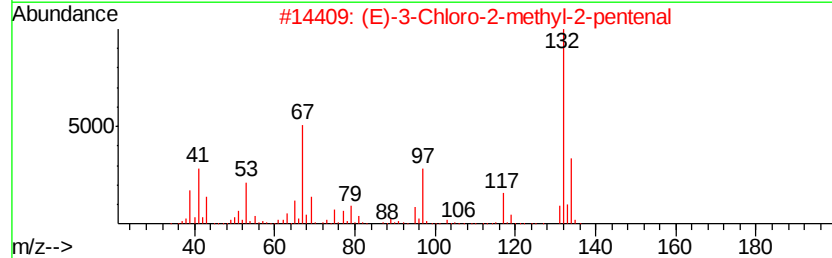
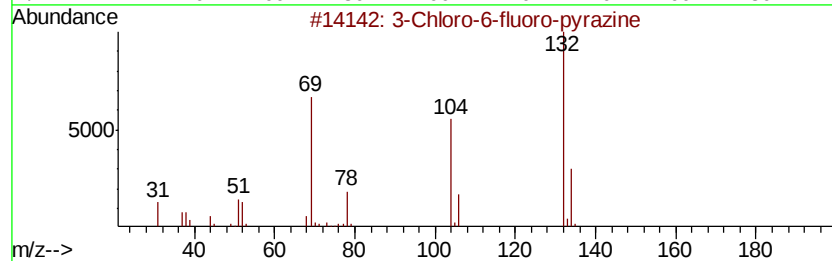
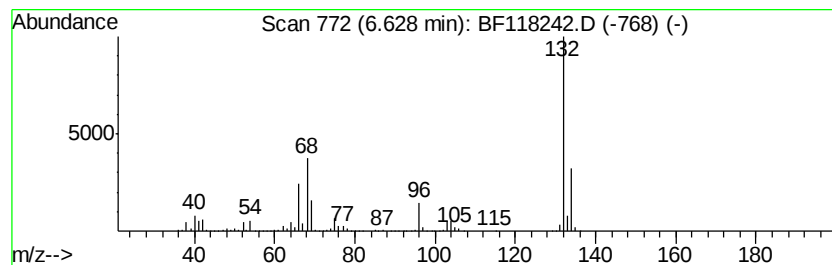
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	69.18 ng	2355640	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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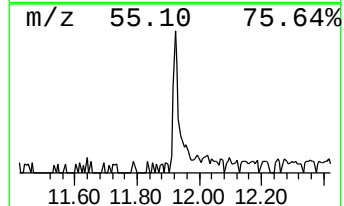
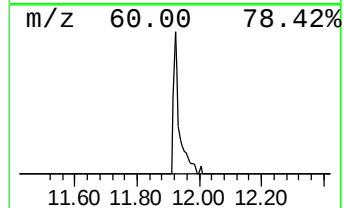
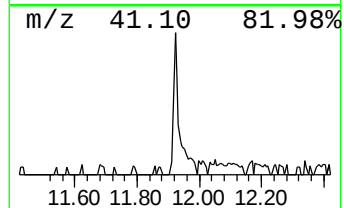
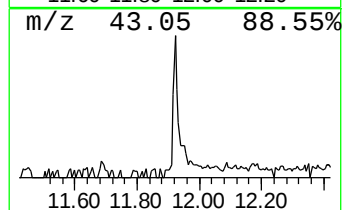
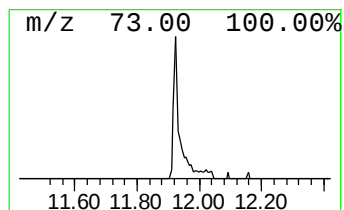
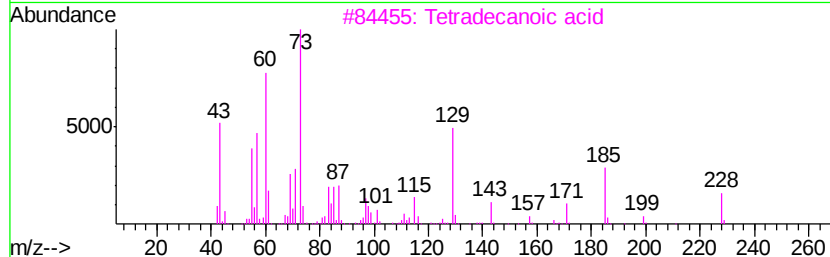
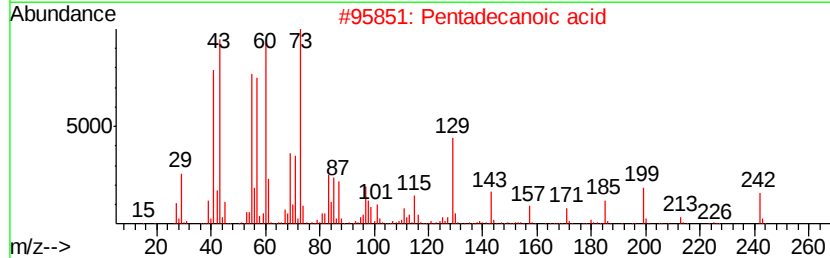
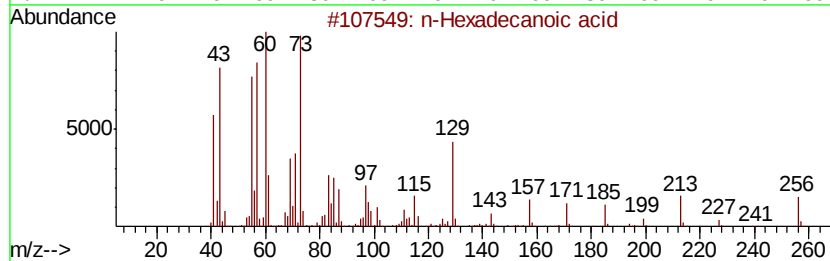
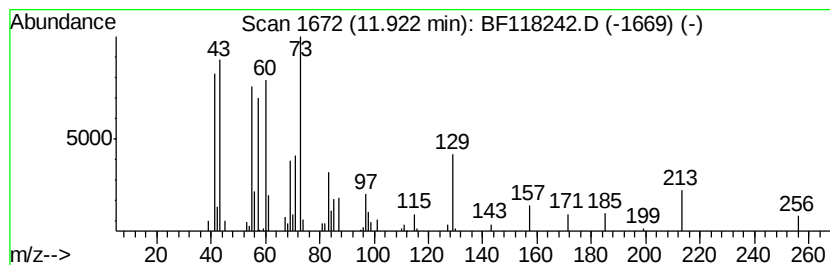
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.37 ng	92279	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	38



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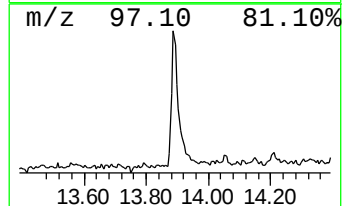
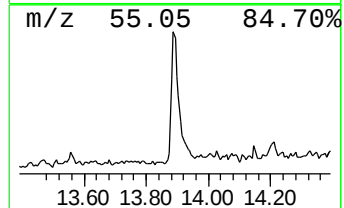
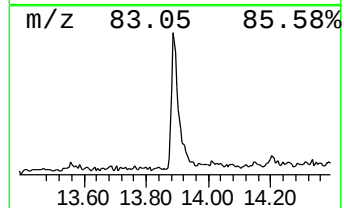
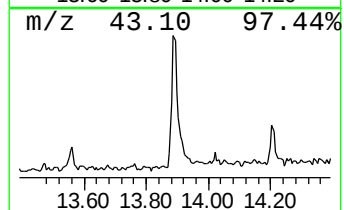
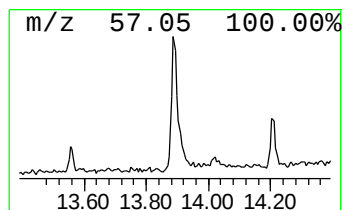
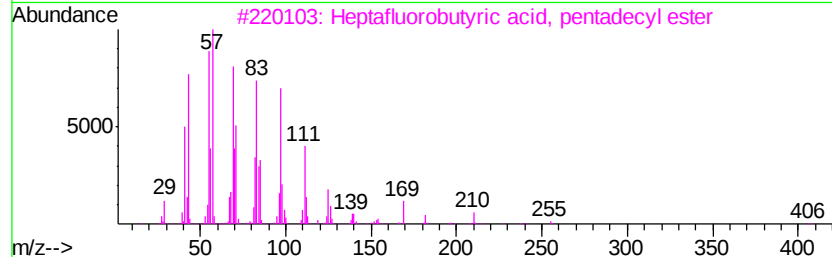
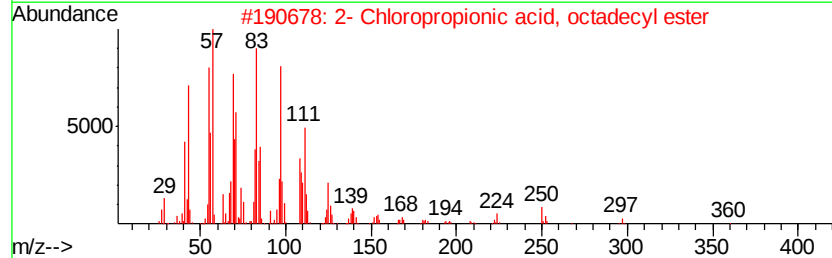
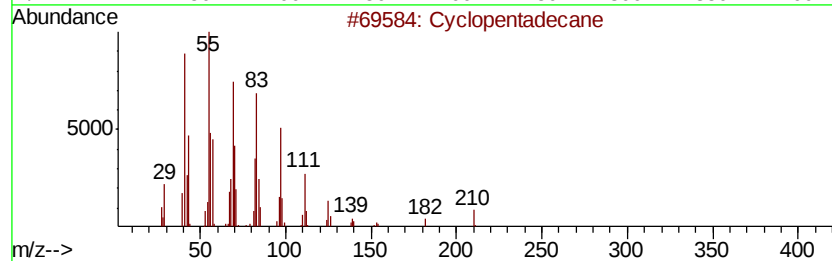
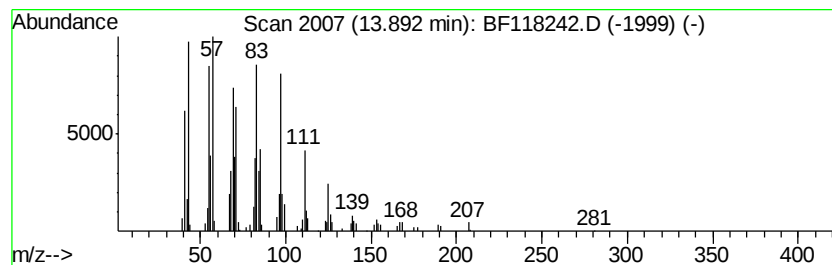
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Peak Number 6 Cyclopentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.89	7.72 ng	283327	Chrysene-d12	14.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvclopentadecane	210	C15H30	000295-48-7	97
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.13	11.4	ng	388543	1	6.86	680992	20.0
2-Pentanone, 4-hy...	5.07	10.5	ng	358713	1	6.86	680992	20.0
unknown6.63	6.63	69.2	ng	2355640	1	6.86	680992	20.0
n-Hexadecanoic acid	11.92	2.4	ng	92279	4	11.40	778477	20.0
Cyclopentadecane	13.89	7.7	ng	283327	5	14.05	733966	20.0