

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050117\
 Data File : BF094786.D
 Acq On : 2 May 2017 8:40
 Operator : SJ/MA
 Sample : I2892-02
 Misc :
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AST-W(2-2.5)

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-BF041717.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	3.937	335	340	354	rBV	452180	607118	19.98%	2.499%
2	4.331	402	407	428	rBV	2573747	2857505	94.06%	11.763%
3	4.707	468	471	478	rVB	35593	41189	1.36%	0.170%
4	5.401	584	589	605	rBV	2553620	2868982	94.43%	11.810%
5	5.519	605	609	615	rVV	2831615	2887197	95.03%	11.885%
6	5.760	647	650	657	rVB	569179	546745	18.00%	2.251%
7	5.943	676	681	684	rBV	2523262	2307644	75.96%	9.500%
8	6.413	756	761	765	rBV	1469142	1650187	54.32%	6.793%
9	7.254	900	904	912	rBV	771479	693209	22.82%	2.854%
10	8.578	1124	1129	1132	rBV	3150930	3038085	100.00%	12.506%
11	9.084	1211	1215	1228	rVB	540462	518992	17.08%	2.136%
12	9.389	1260	1267	1276	rBV2	705614	712205	23.44%	2.932%
13	9.983	1365	1368	1372	rBV	41377	36495	1.20%	0.150%
14	10.372	1429	1434	1446	rBV	1250071	1441996	47.46%	5.936%
15	10.572	1464	1468	1470	rBV	47768	57144	1.88%	0.235%
16	11.125	1557	1562	1565	rBV	34017	31861	1.05%	0.131%
17	11.213	1573	1577	1585	rBV	575926	568366	18.71%	2.340%
18	11.948	1698	1702	1708	rBV3	36275	49022	1.61%	0.202%
19	13.024	1881	1885	1892	rBV2	67706	67538	2.22%	0.278%
20	13.195	1908	1914	1917	rBV	2014180	2256339	74.27%	9.288%
21	13.901	2030	2034	2037	rBV	50399	45062	1.48%	0.186%
22	14.418	2117	2122	2126	rBV7	16435	37967	1.25%	0.156%
23	14.466	2126	2130	2134	rVV	527718	540232	17.78%	2.224%
24	16.095	2403	2407	2414	rVB	390238	431077	14.19%	1.775%

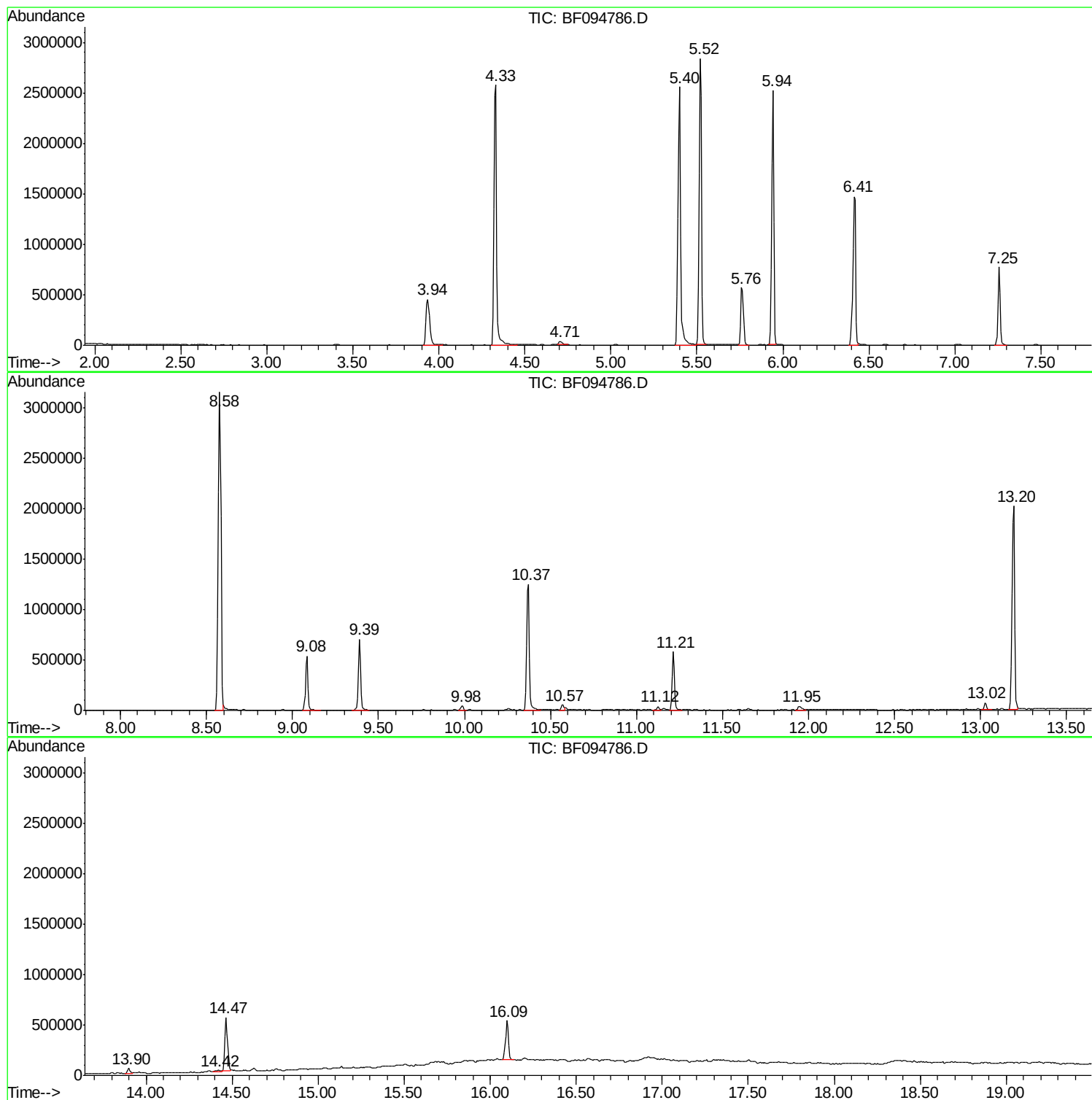
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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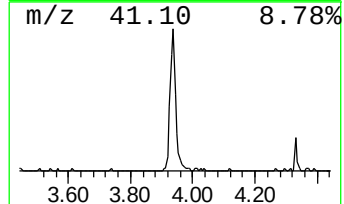
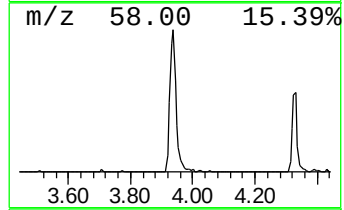
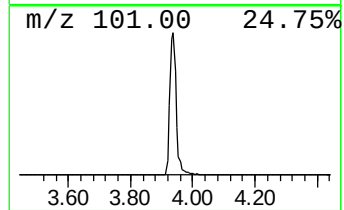
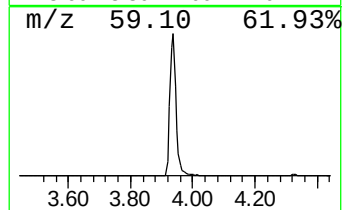
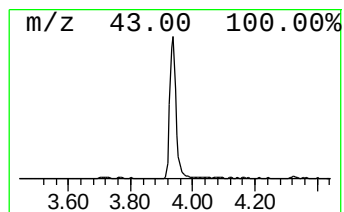
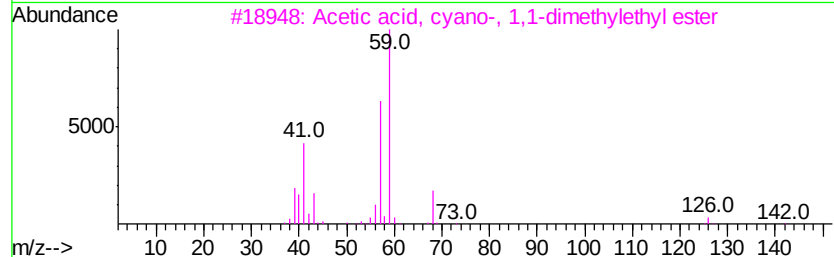
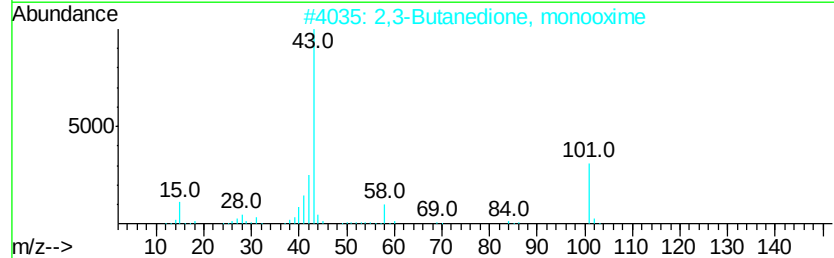
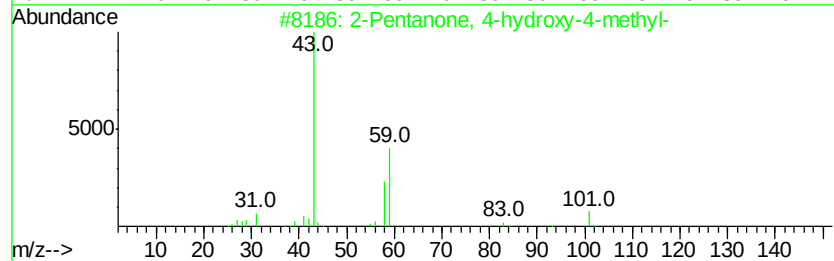
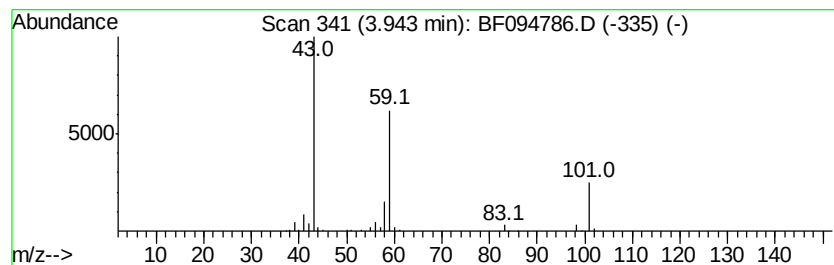
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.94	22.21 ng	607118	1,4-Dichlorobenzene-d4	5.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9



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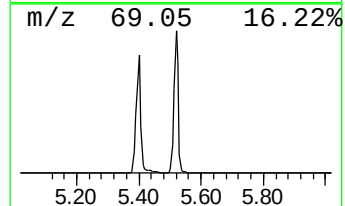
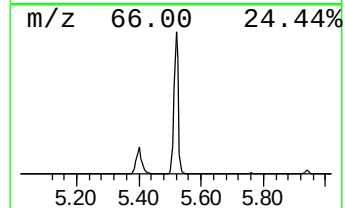
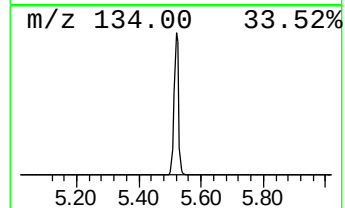
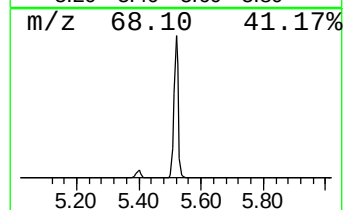
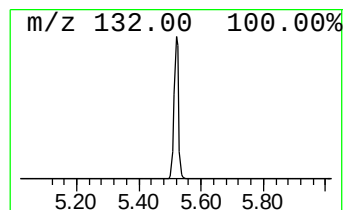
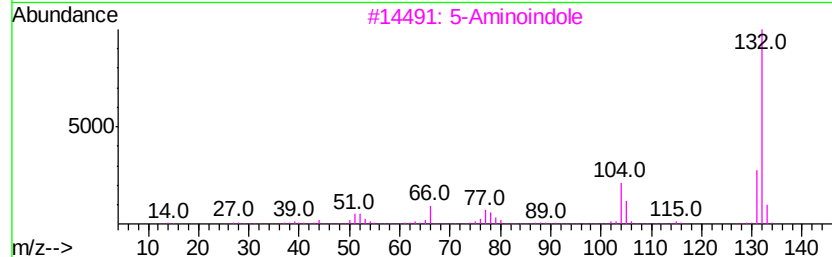
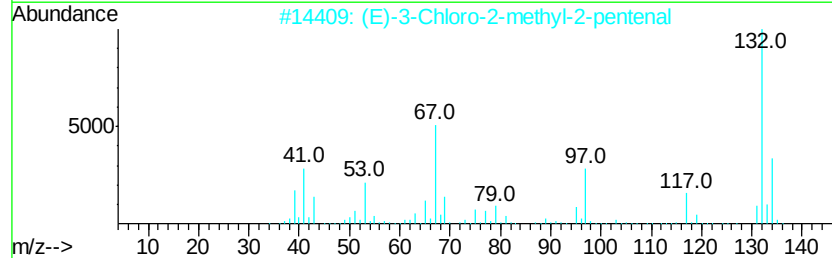
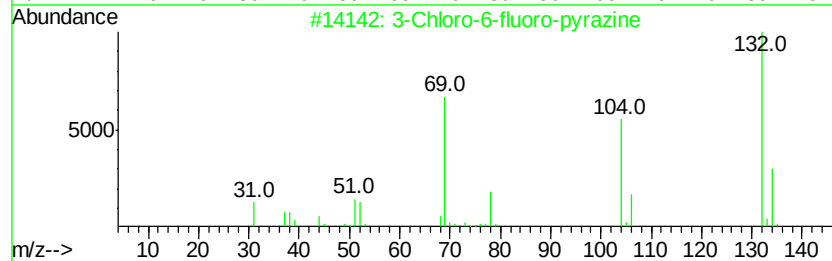
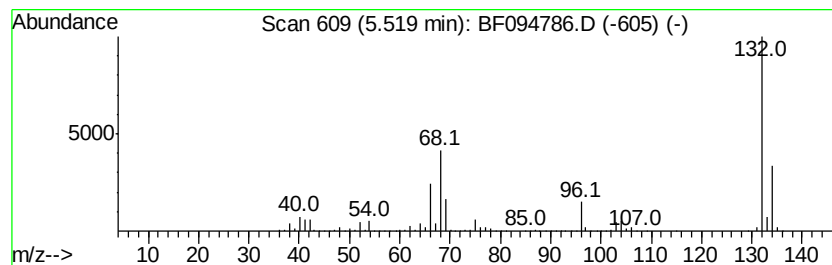
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Peak Number 2 unknown5.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.52	105.61 ng	2887200	1,4-Dichlorobenzene-d4	5.77

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	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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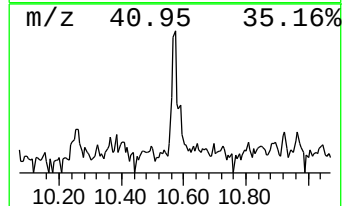
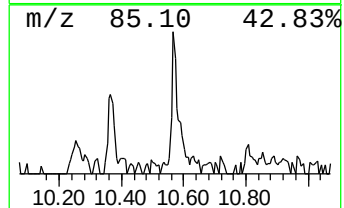
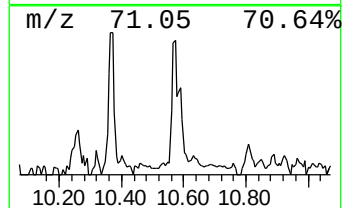
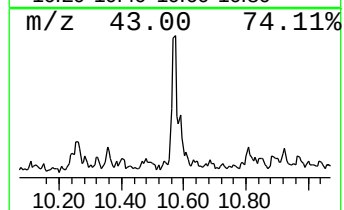
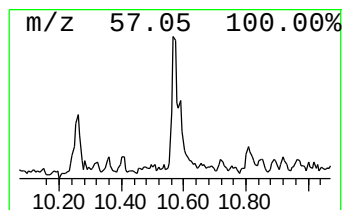
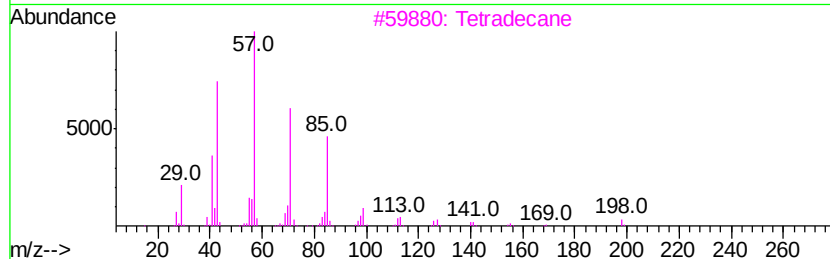
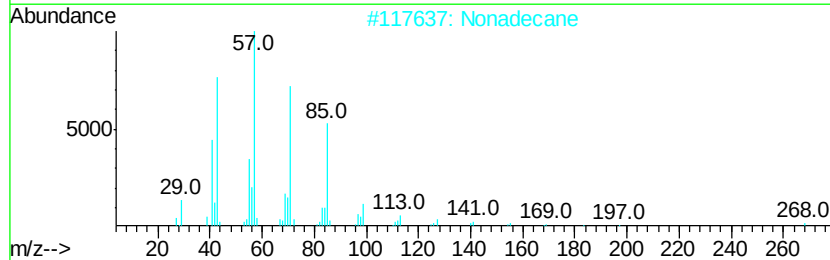
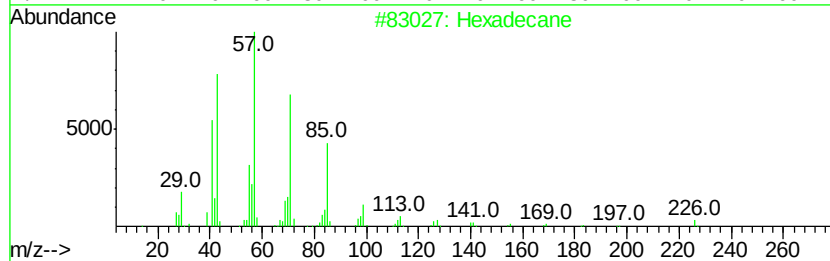
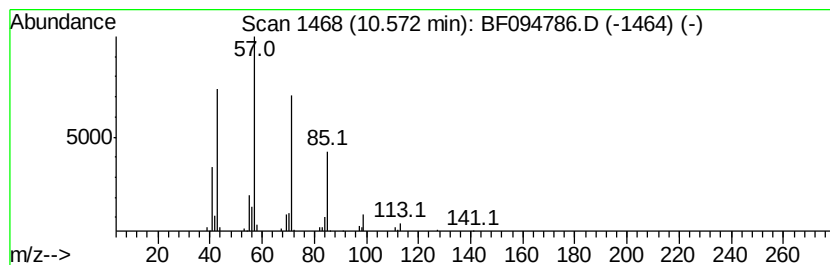
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
10.57	2.01 ng	57144	Phenanthrene-d10		11.21		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	91
2			Nonadecane	268	C19H40	000629-92-5	91
3			Tetradecane	198	C14H30	000629-59-4	90
4			Hexacosane	366	C26H54	000630-01-3	90
5			Pentadecane	212	C15H32	000629-62-9	90



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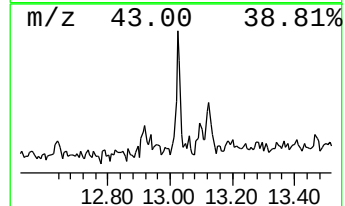
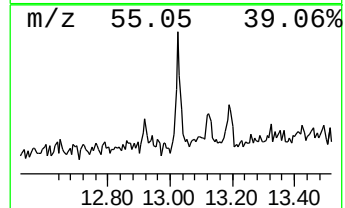
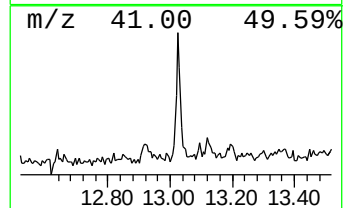
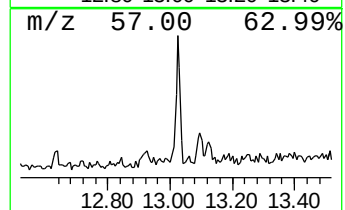
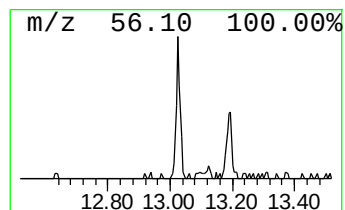
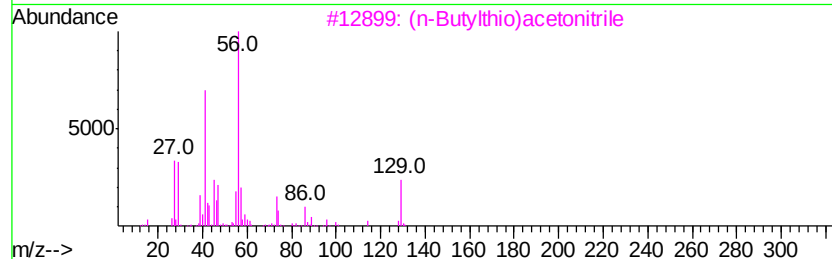
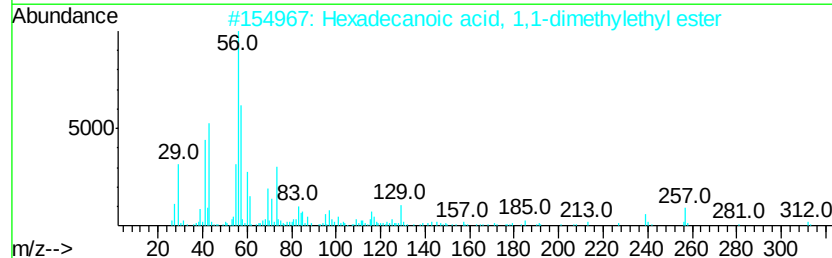
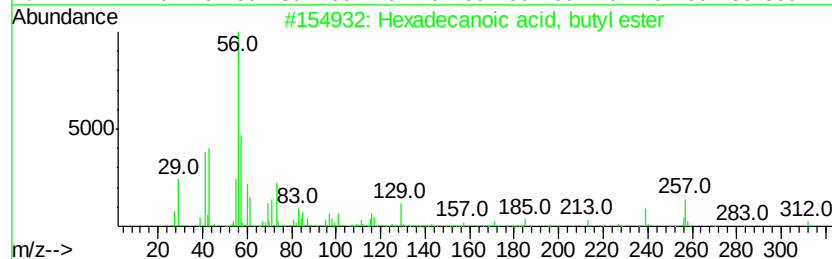
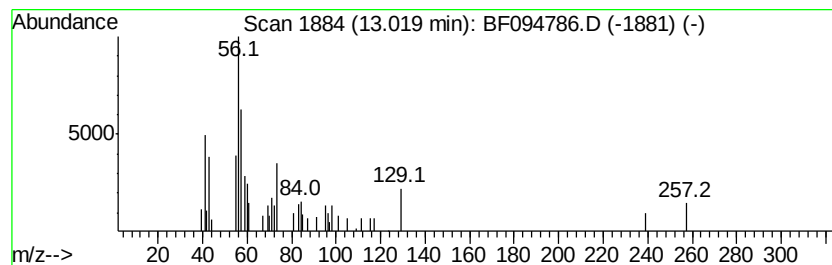
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.02	2.50 ng	67538	Chrysene-d12	14.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
3		(n-Butylthio)acetonitrile	129	C6H11NS	071037-08-6	49
4		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	3.94	22.2	ng	607118	1	5.77	546745	20.0
unknown5.52	5.52	105.6	ng	2887200	1	5.77	546745	20.0
Hexadecane	10.57	2.0	ng	57144	4	11.21	568366	20.0
Hexadecanoic acid...	13.02	2.5	ng	67538	5	14.47	540232	20.0