

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093657.D
 Acq On : 14 Mar 2017 14:31
 Operator : SJ/MA
 Sample : I2224-01
 Misc :
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 030917-PRRT-F-U-M

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-BF030717.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	4.847	257	259	267	rBV	313523	568134	11.71%	1.784%
2	4.950	267	268	277	rVB2	19460	57109	1.18%	0.179%
3	5.316	297	300	329	rBV	603309	1473588	30.37%	4.628%
4	6.379	391	393	400	rBV	518791	961624	19.82%	3.020%
5	6.481	400	402	417	rVV	2182649	2803149	57.76%	8.804%
6	6.710	420	422	430	rVB	966427	1072510	22.10%	3.368%
7	6.859	433	435	444	rBV	3314627	3585185	73.88%	11.260%
8	7.282	470	472	487	rBV	2542910	3179651	65.52%	9.986%
9	8.002	533	535	547	rVB	1314745	1368812	28.21%	4.299%
10	9.076	627	629	632	rBV	3650912	4852905	100.00%	15.241%
11	9.499	663	666	674	rBV	65547	96710	1.99%	0.304%
12	9.762	686	689	691	rBV	1215175	1469337	30.28%	4.615%
13	10.550	756	758	766	rBV	1649159	1862127	38.37%	5.848%
14	10.665	766	768	772	rVB	77002	97295	2.00%	0.306%
15	11.110	805	807	808	rBV	58621	49378	1.02%	0.155%
16	11.248	817	819	825	rBV	1545540	1549204	31.92%	4.865%
17	12.653	939	942	944	rBV	165453	163099	3.36%	0.512%
18	12.836	955	958	960	rBV	3266447	4407793	90.83%	13.843%
19	13.351	1001	1003	1005	rBV	131097	108258	2.23%	0.340%
20	13.888	1048	1050	1060	rVB	1116382	1241879	25.59%	3.900%
21	15.294	1170	1173	1185	rVB	530817	872860	17.99%	2.741%

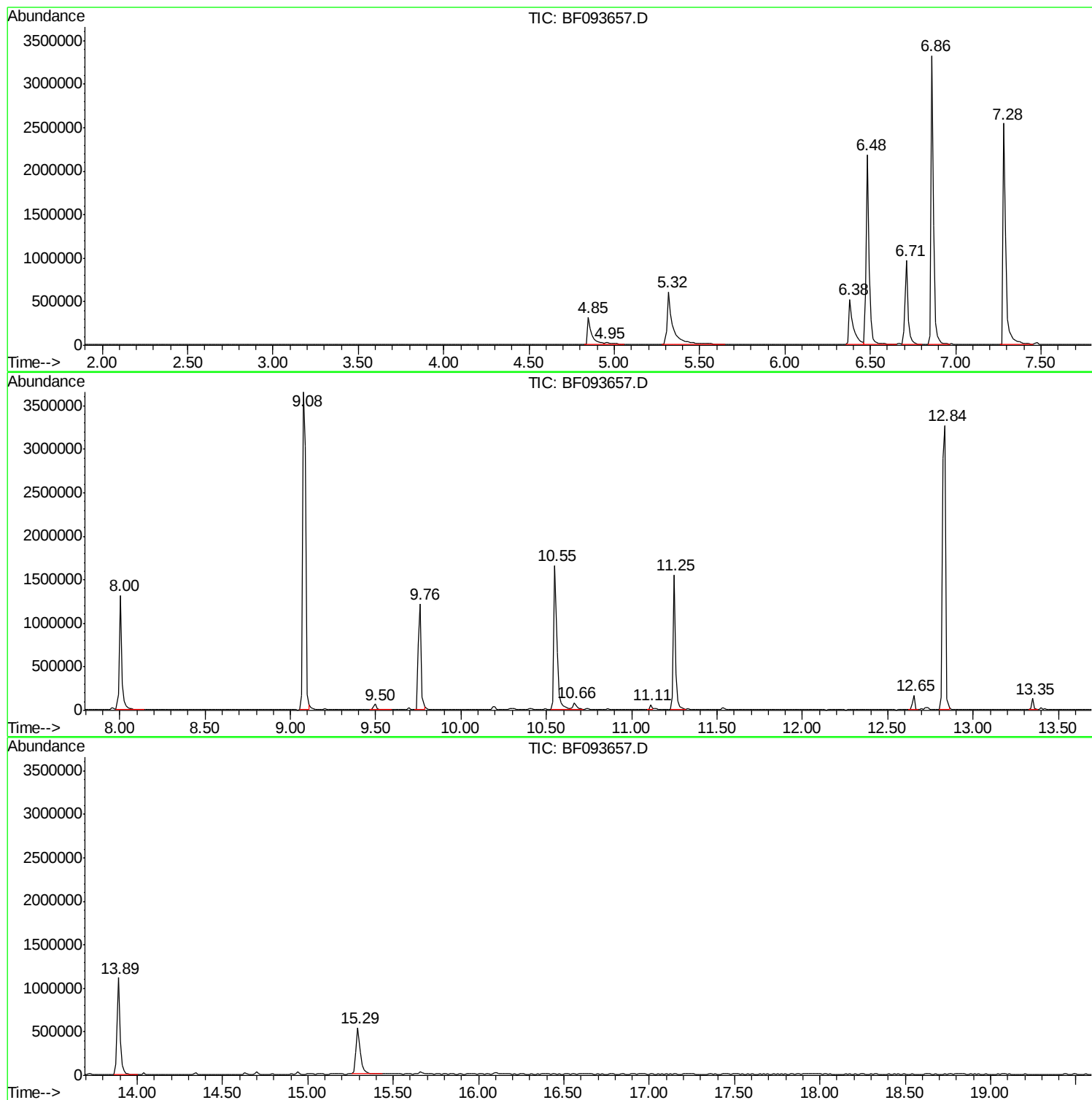
Sum of corrected areas: 31840607

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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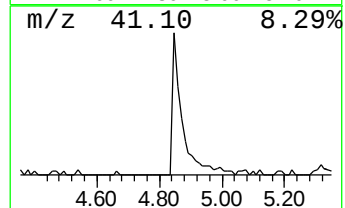
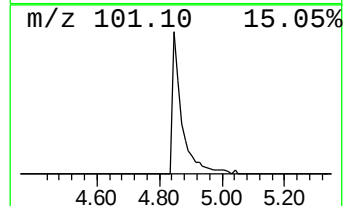
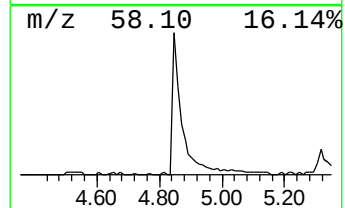
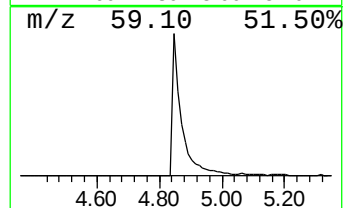
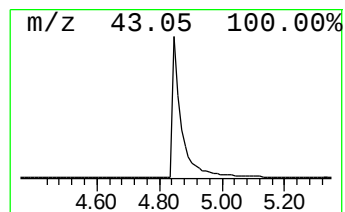
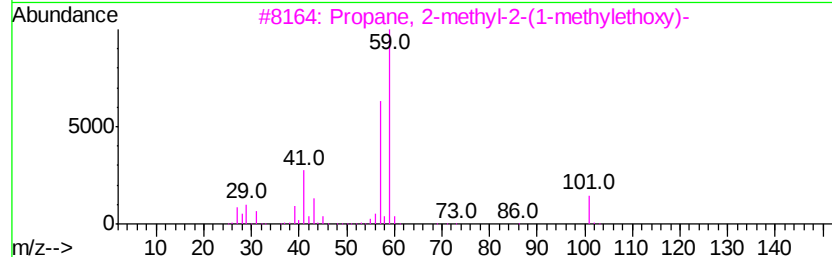
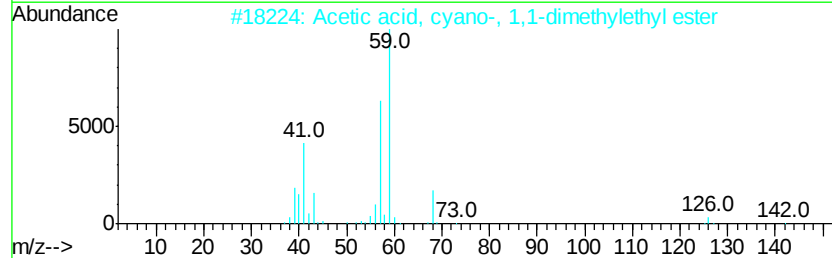
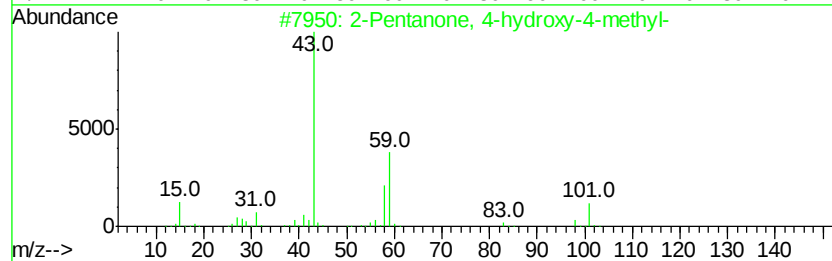
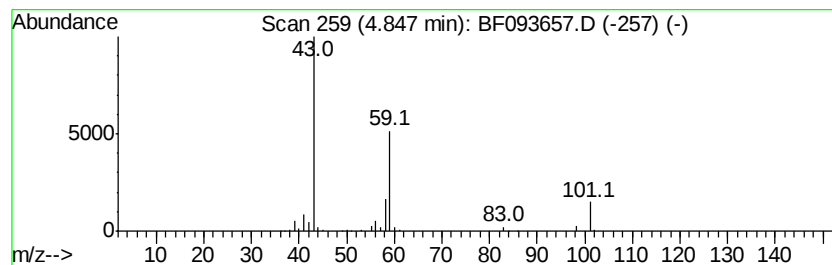
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.85	10.59 ng	568134	1,4-Dichlorobenzene-d4	6.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	37
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Octanol	130	C8H18O	000589-98-0	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33



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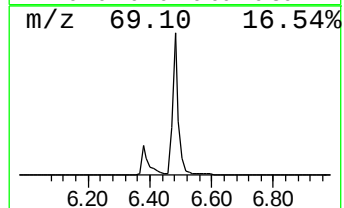
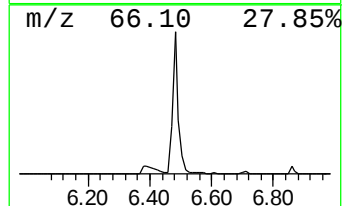
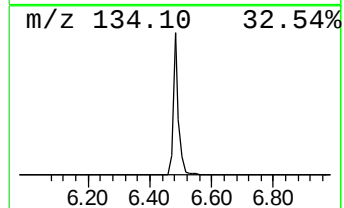
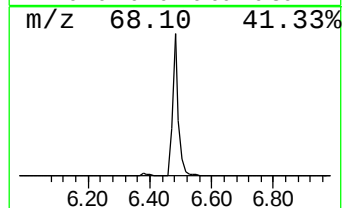
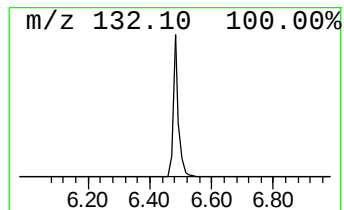
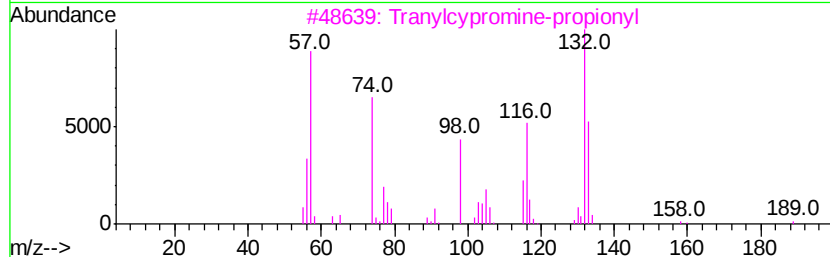
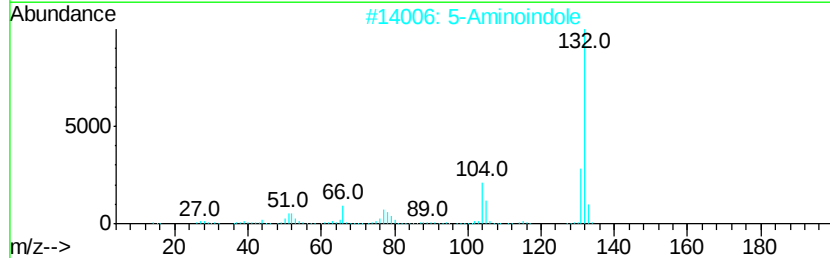
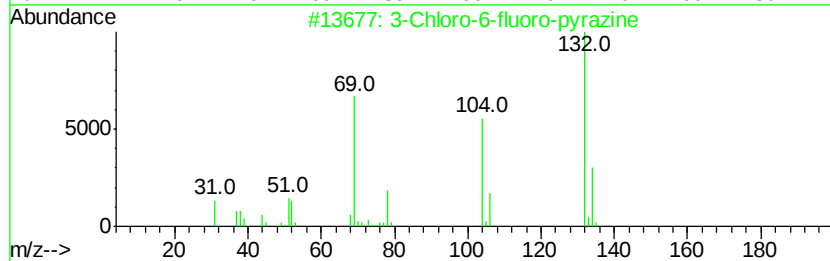
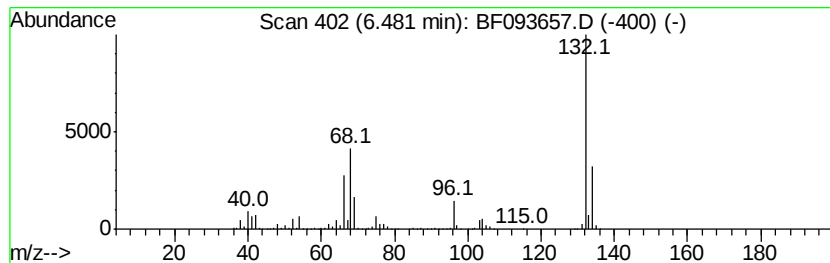
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Peak Number 2 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	52.27 ng	2803150	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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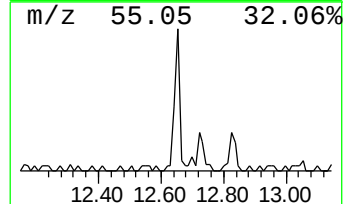
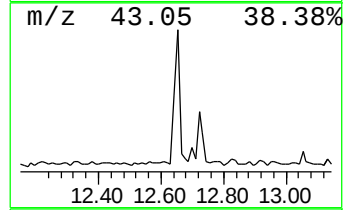
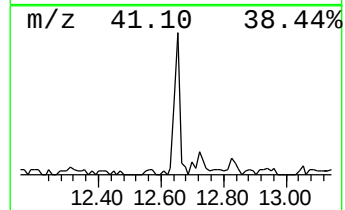
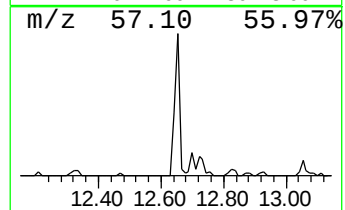
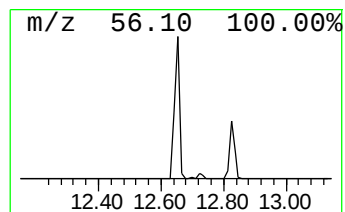
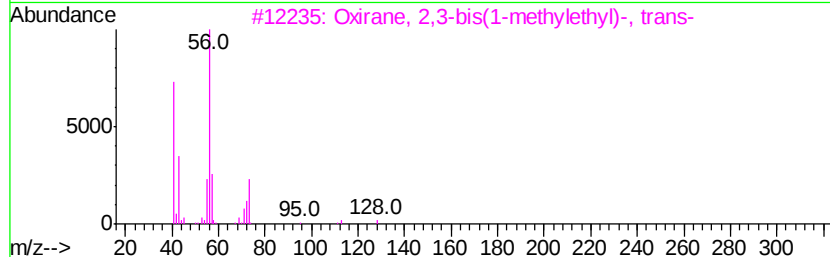
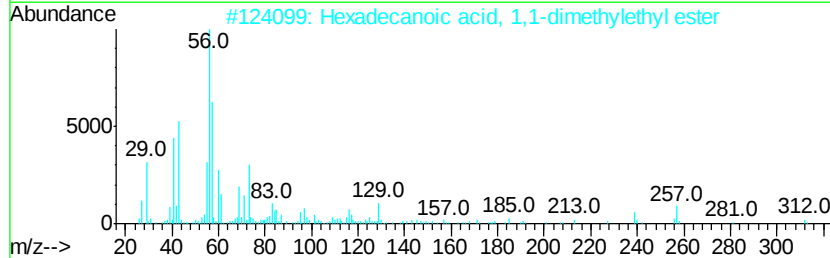
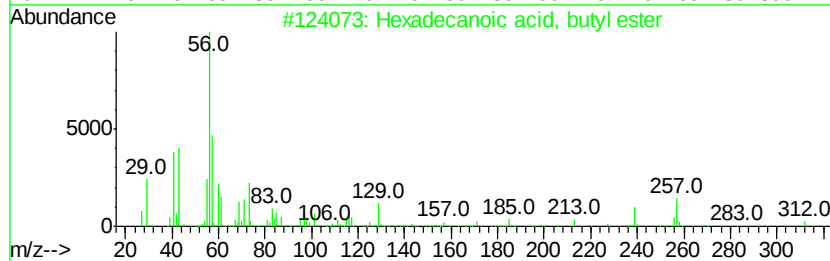
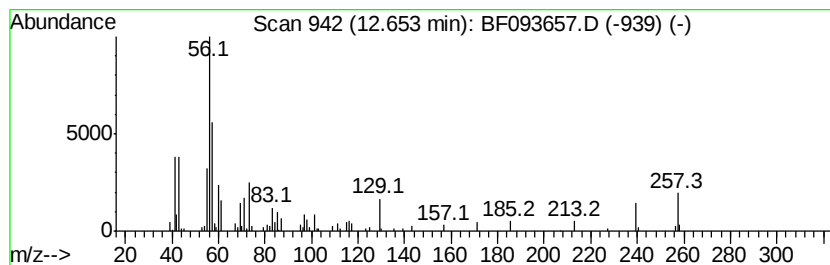
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Peak Number 4 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.63 ng	163099	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	43
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
4		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.85	10.6	ng	568134	1	6.71	1072510	20.0
unknown6.48	6.48	52.3	ng	2803150	1	6.71	1072510	20.0
Hexadecanoic acid...	12.65	2.6	ng	163099	5	13.89	1241880	20.0