

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101817\
 Data File : BG029343.D
 Acq On : 18 Oct 2017 22:31
 Operator : SJ/JU
 Sample : I5834-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-115-4(30-40)

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_G\METHODS\8270-BG101617.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	5.245	327	333	342	rVB	222401	332056	6.51%	1.274%
2	5.721	406	414	424	rBV	1143328	1821638	35.69%	6.990%
3	7.325	678	687	699	rBV	1122085	2091946	40.98%	8.028%
4	7.701	742	751	765	rBV	1095891	1926894	37.75%	7.394%
5	8.165	823	830	838	rBV	202960	349463	6.85%	1.341%
6	8.494	878	886	895	rVB	822929	1431989	28.05%	5.495%
7	9.334	1020	1029	1039	rBV	651433	1188388	23.28%	4.560%
8	10.985	1302	1310	1318	rVB	289009	528379	10.35%	2.028%
9	13.412	1715	1723	1734	rBV	1892913	2895127	56.72%	11.110%
10	14.229	1852	1862	1868	rBV	360323	541981	10.62%	2.080%
11	14.787	1950	1957	1965	rVB2	490825	807340	15.82%	3.098%
12	16.126	2181	2185	2191	rVB	68330	96662	1.89%	0.371%
13	16.267	2202	2209	2219	rBV	1855009	2847914	55.79%	10.928%
14	17.519	2415	2422	2431	rBV2	710292	1128818	22.11%	4.332%
15	18.388	2566	2570	2580	rBV3	69318	122046	2.39%	0.468%
16	20.116	2857	2864	2870	rBV	3729309	5104375	100.00%	19.587%
17	21.790	3142	3149	3157	rVB2	868623	1421991	27.86%	5.457%
18	25.098	3701	3712	3725	rVB	496842	1422574	27.87%	5.459%

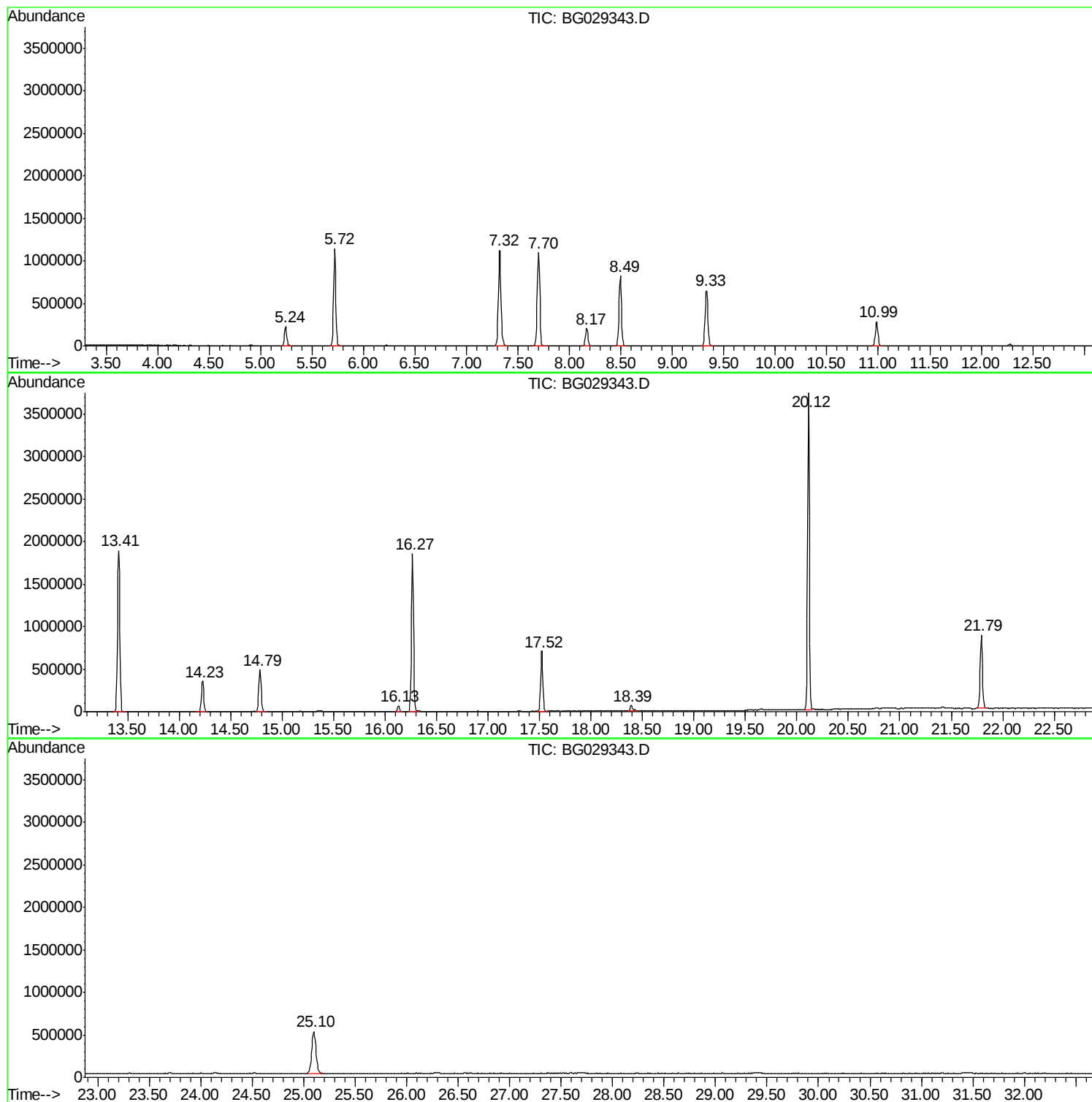
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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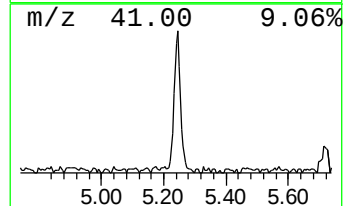
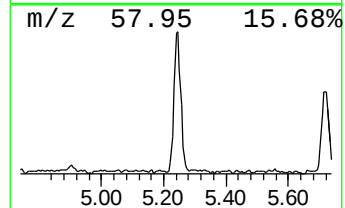
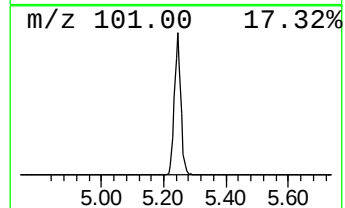
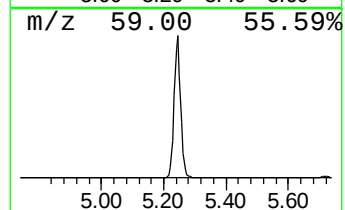
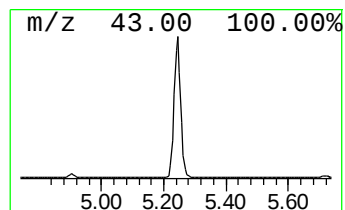
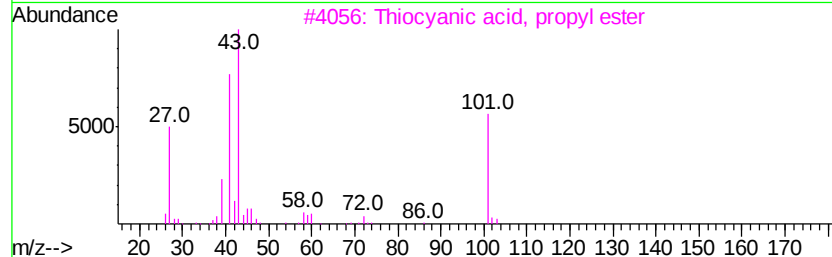
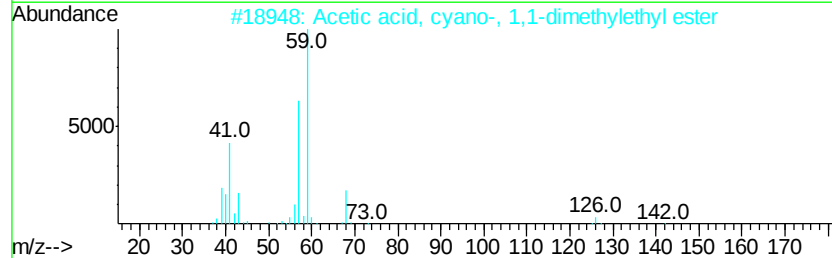
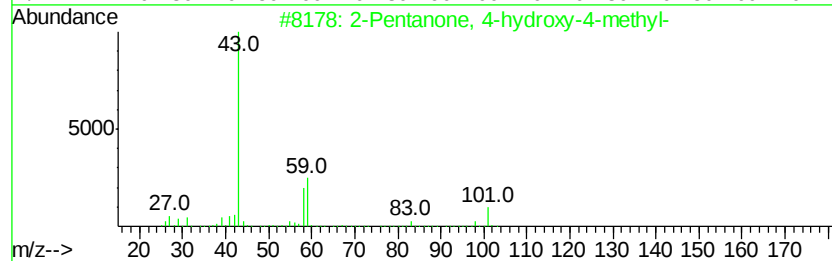
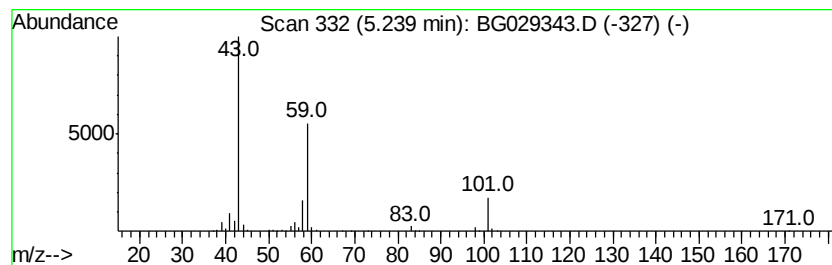
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	19.00 ng	332056	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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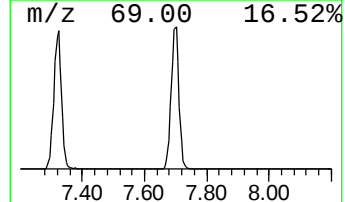
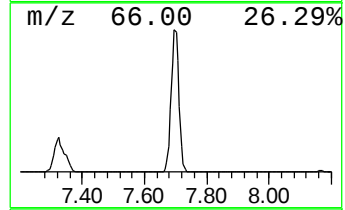
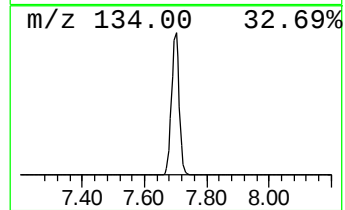
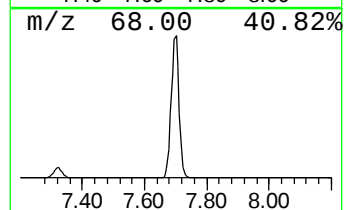
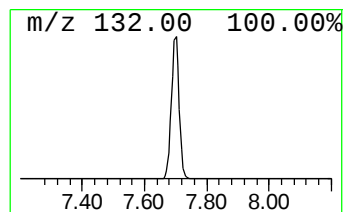
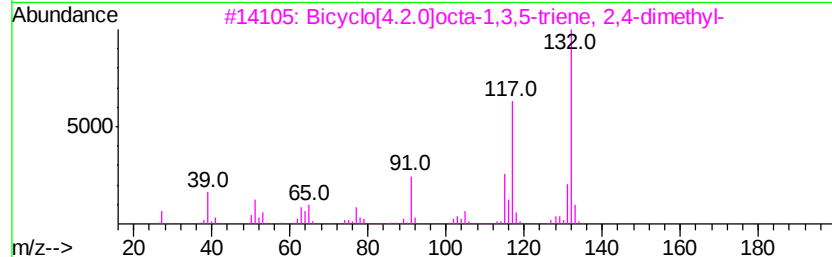
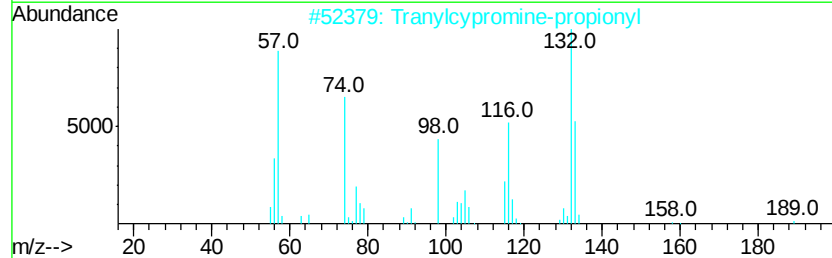
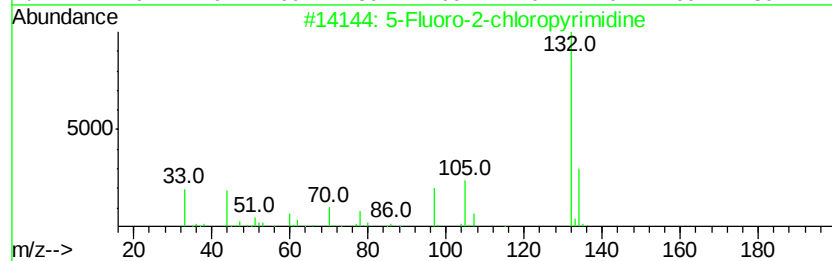
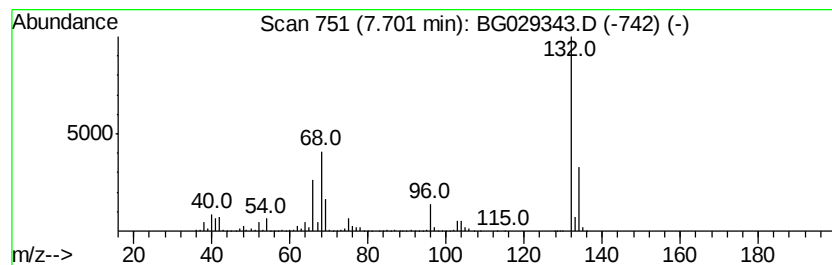
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Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	110.28 ng	1926890	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		Xenon	132	Xe	007440-63-3	9



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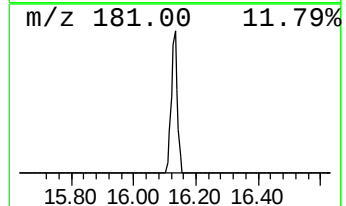
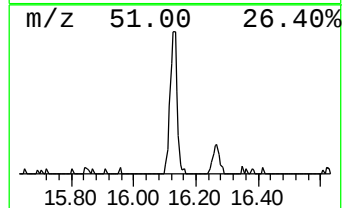
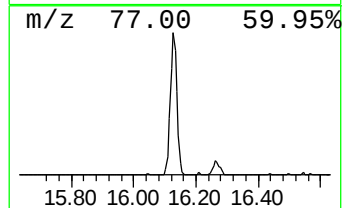
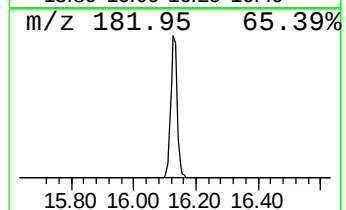
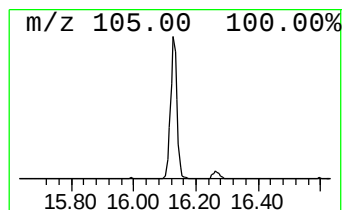
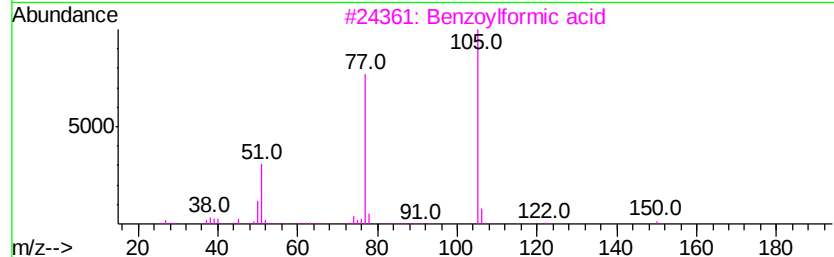
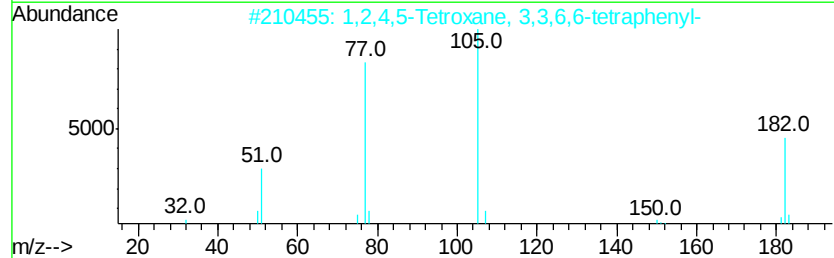
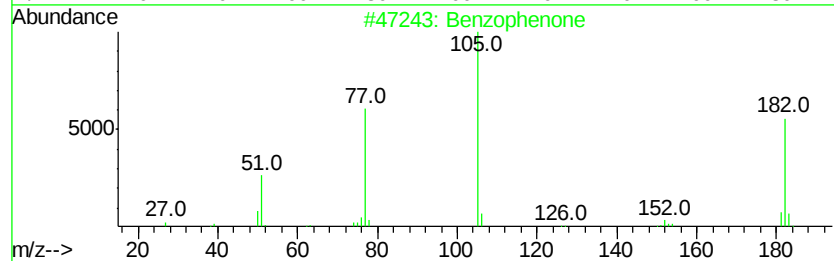
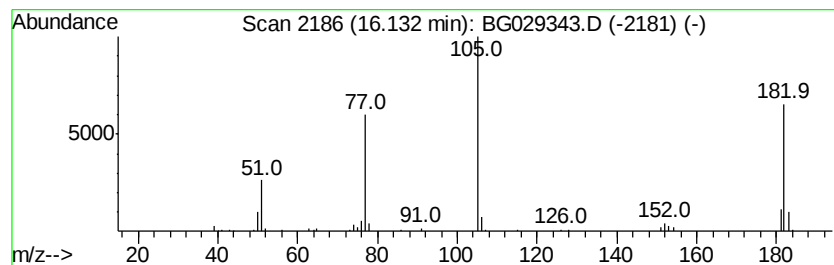
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Peak Number 4 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.39 ng	96662	Acenaphthene-d10	14.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	97
2		1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3		Benzoylformic acid	150	C8H6O3	000611-73-4	55
4		Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5		Ethanone, 2,2-dihydroxy-1-phenyl-	152	C8H8O3	001075-06-5	46



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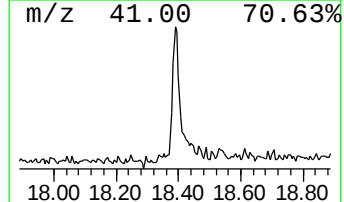
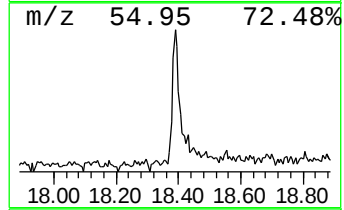
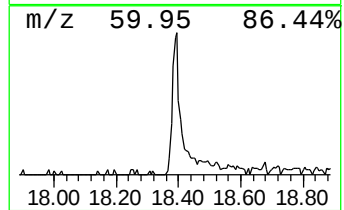
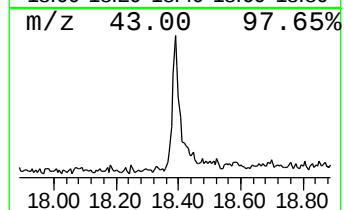
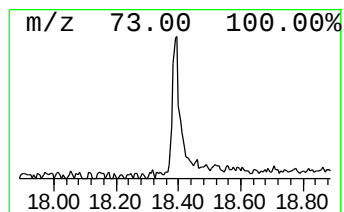
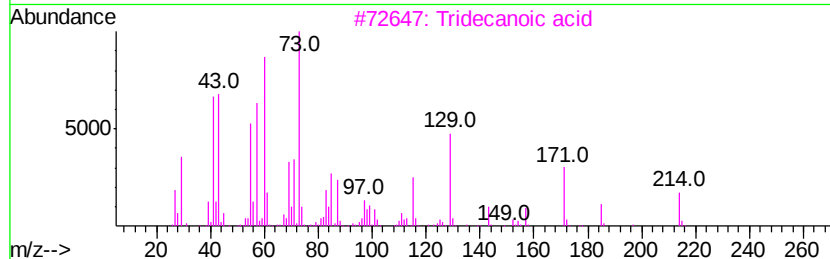
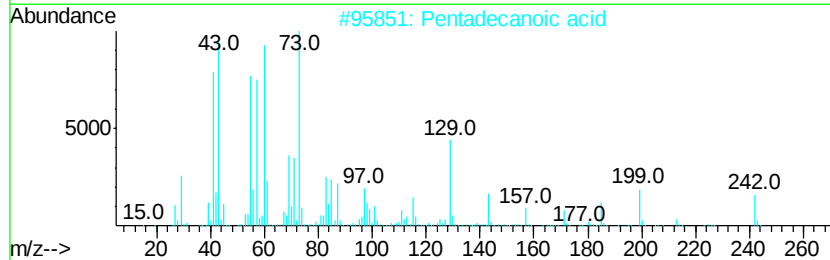
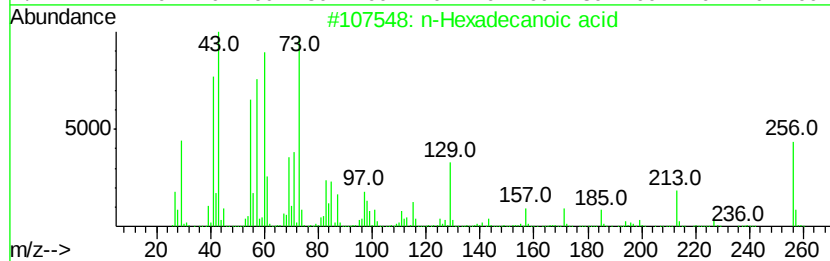
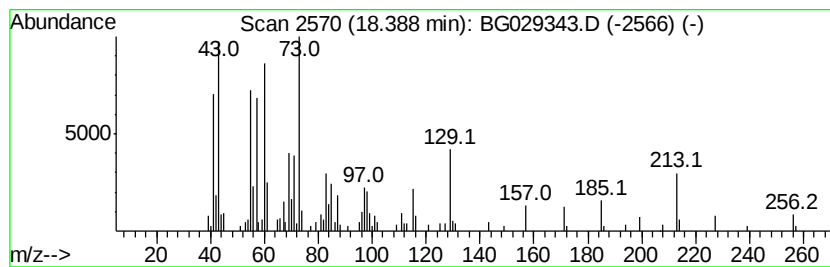
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.16 ng	122046	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.24	19.0	ng	332056	1	8.17	349463	20.0
unknown7.70	7.70	110.3	ng	1926890	1	8.17	349463	20.0
Benzophenone	16.13	2.4	ng	96662	3	14.78	807340	20.0
n-Hexadecanoic acid	18.39	2.2	ng	122046	4	17.52	1128820	20.0