

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081616\
 Data File : BF089757.D
 Acq On : 17 Aug 2016 11:45
 Operator : UM/SJ
 Sample : H4429-04
 Misc :
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LOCATION-29A-9-11

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:\HPCHEM1\BNA_F\METHODS\8270-BF081616.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	1.667	6	7	16	rVV	1863512	3115901	16.45%	1.758%
2	1.793	16	18	28	rVV	9852143	18936333	100.00%	10.685%
3	1.918	28	29	66	rVB	818573	3842163	20.29%	2.168%
4	4.856	283	286	295	rBV	1917198	3108226	16.41%	1.754%
5	5.290	320	324	326	rBV	9358659	13621326	71.93%	7.686%
6	6.330	412	415	418	rBV	9274949	12660835	66.86%	7.144%
7	6.467	424	427	429	rBV	12697151	14250910	75.26%	8.041%
8	6.696	445	447	450	rBV	4947864	4349260	22.97%	2.454%
9	6.856	458	461	463	rBV	11998957	10841812	57.25%	6.118%
10	7.267	493	497	499	rBV	7751946	9337117	49.31%	5.269%
11	7.736	534	538	541	rBV2	216992	311762	1.65%	0.176%
12	7.988	557	560	562	rBV	6087954	6200214	32.74%	3.499%
13	9.073	651	655	657	rBV	11434129	16765442	88.54%	9.460%
14	9.462	687	689	691	rVB	4152601	3412214	18.02%	1.925%
15	9.736	710	713	715	rBV	7861010	6950766	36.71%	3.922%
16	10.193	748	753	754	rBV	222501	282585	1.49%	0.159%
17	10.411	768	772	775	rBV	114666	191045	1.01%	0.108%
18	10.525	779	782	784	rBV2	6928564	9503396	50.19%	5.362%
19	10.662	792	794	800	rVB	485413	547676	2.89%	0.309%
20	11.211	840	842	845	rVB	7692771	6712476	35.45%	3.788%
21	11.759	888	890	896	rBV2	553791	945671	4.99%	0.534%
22	12.559	958	960	967	rBV	274130	364817	1.93%	0.206%
23	12.822	980	983	986	rBV	11249128	15263475	80.60%	8.613%
24	13.954	1079	1082	1086	rBV2	7191455	10510534	55.50%	5.931%
25	14.102	1087	1095	1098	rVV7	36003	226780	1.20%	0.128%
26	15.543	1217	1221	1223	rBV	3682100	4966790	26.23%	2.803%

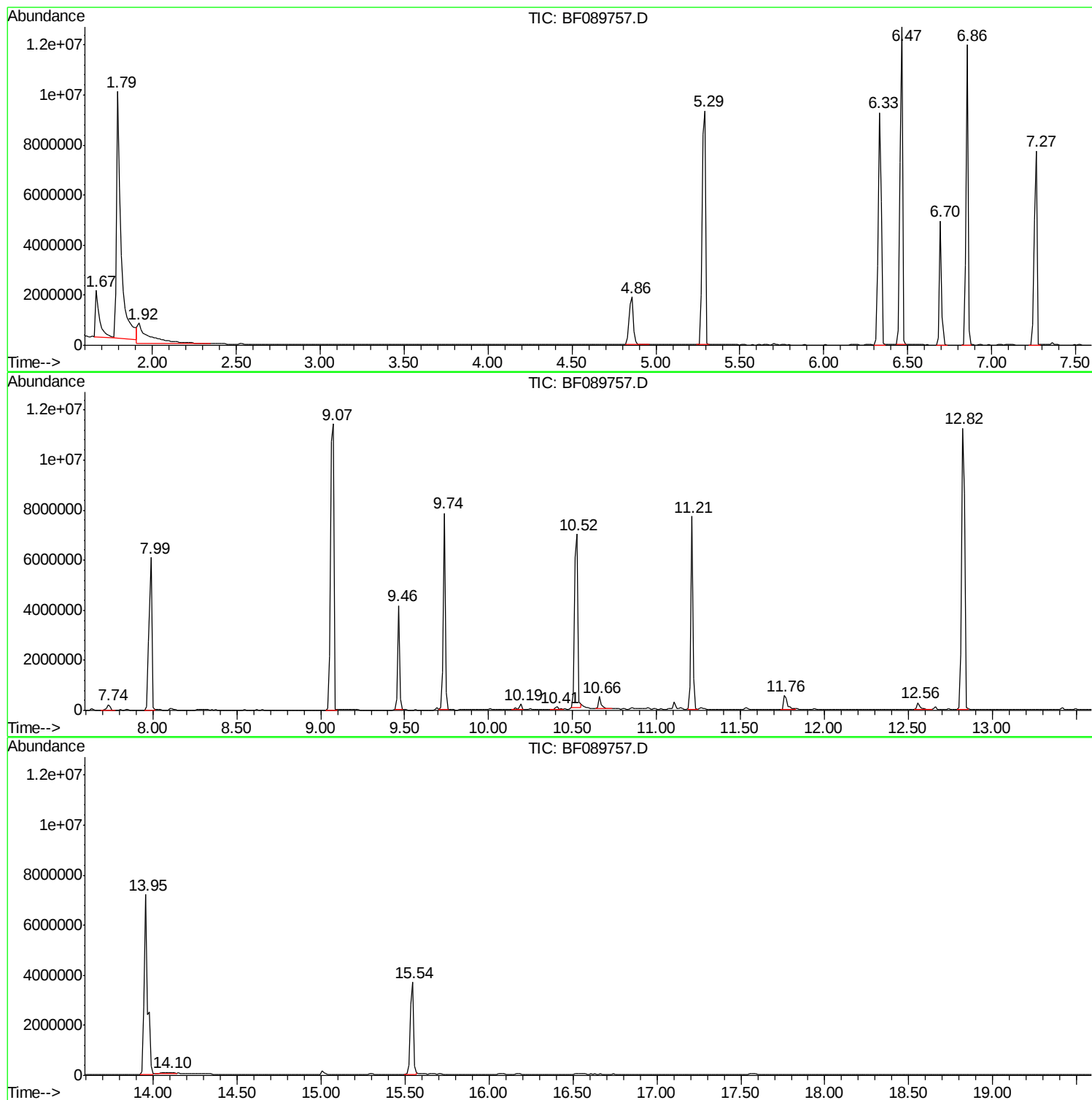
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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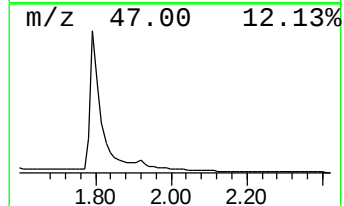
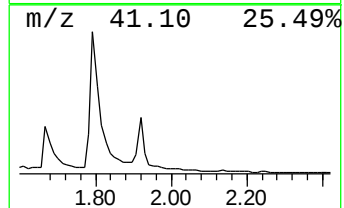
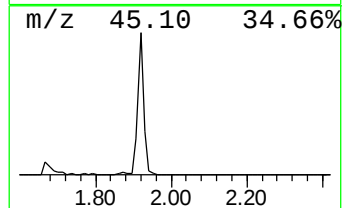
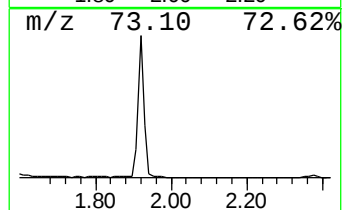
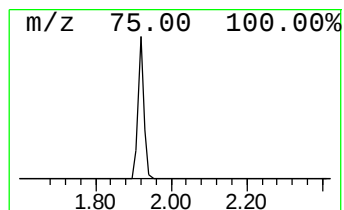
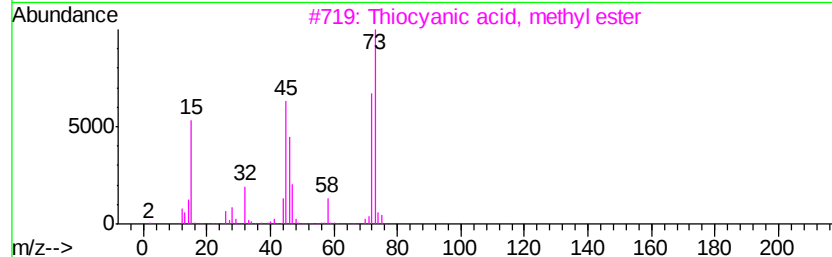
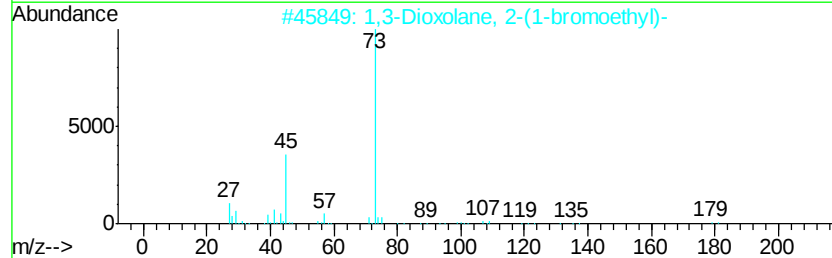
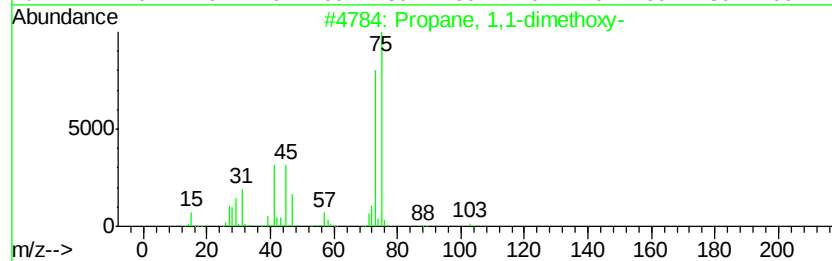
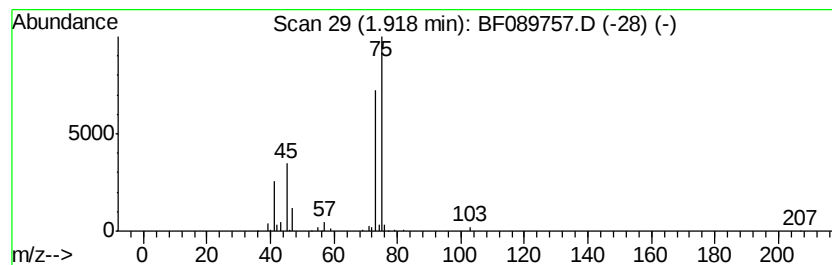
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.92	17.67 ng	3842160	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2		1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	14
3		Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	14
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		Acetic acid, (aminooxy)-	91	C2H5NO3	000645-88-5	9



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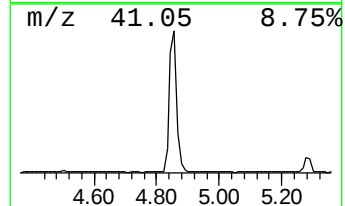
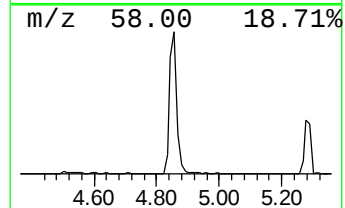
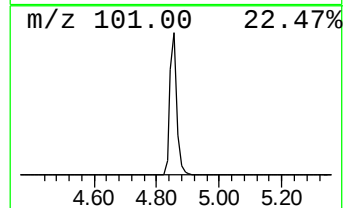
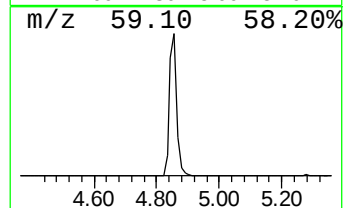
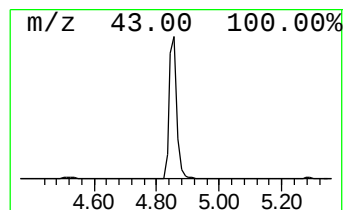
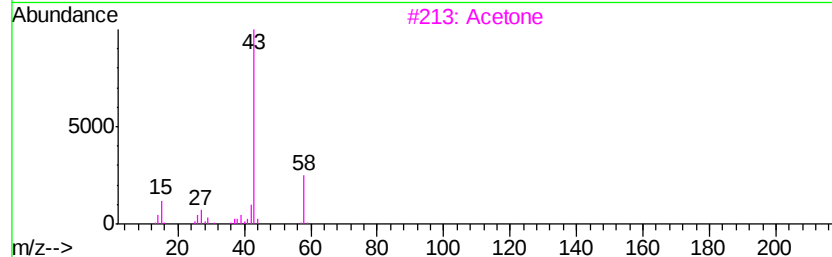
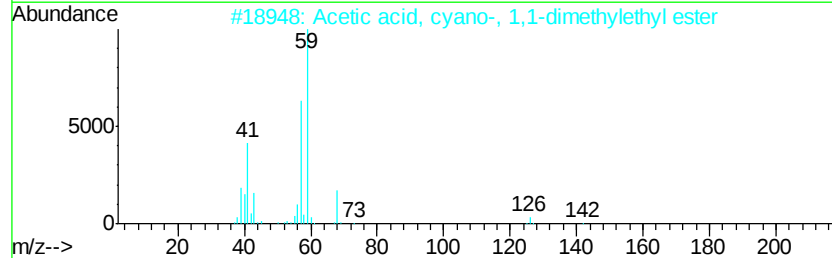
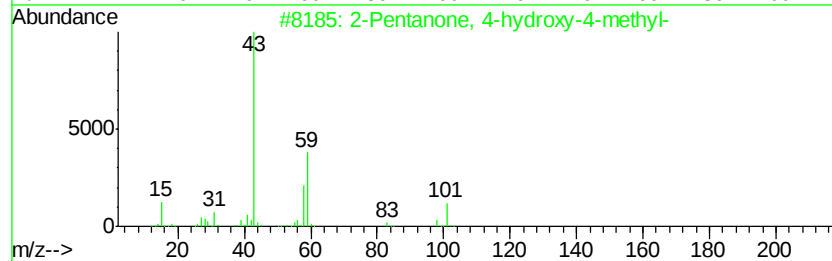
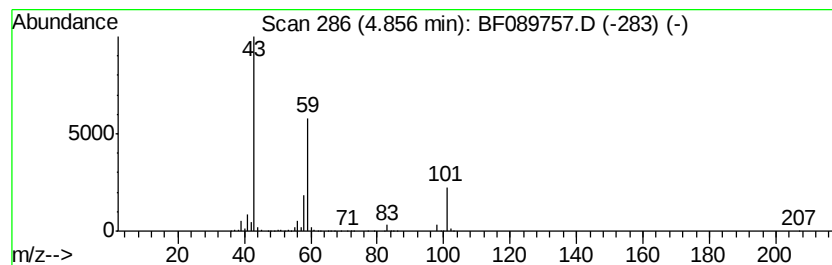
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	14.29 ng	3108230	1,4-Dichlorobenzene-d4	6.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Acetone	58	C3H6O	000067-64-1	9	
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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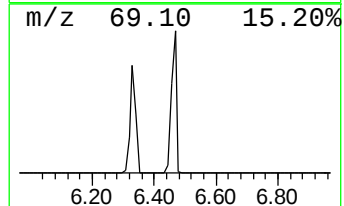
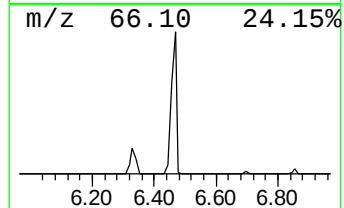
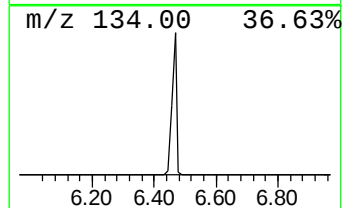
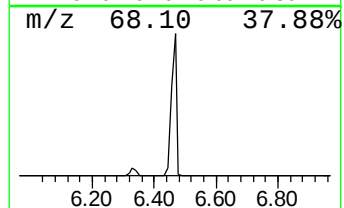
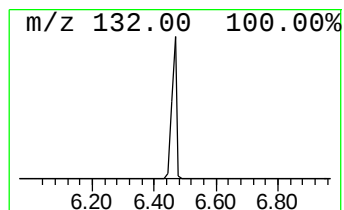
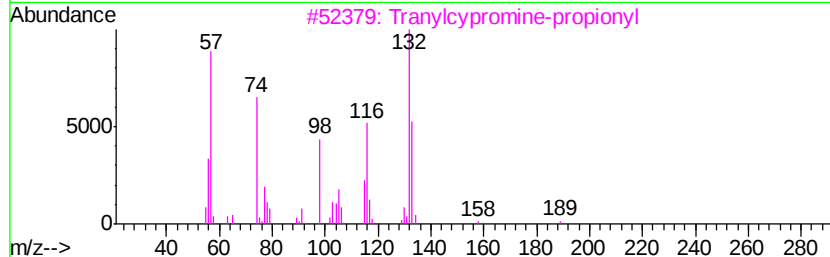
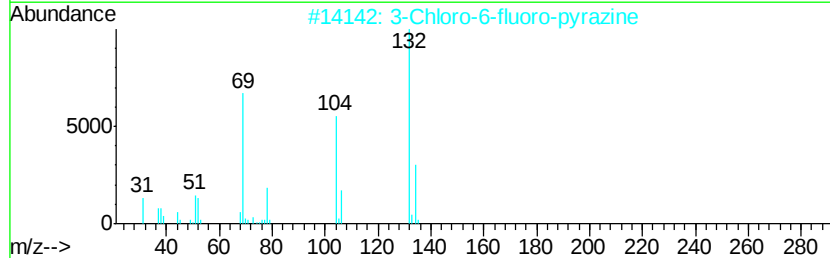
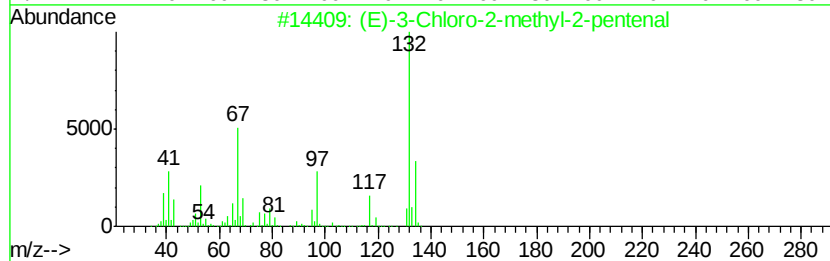
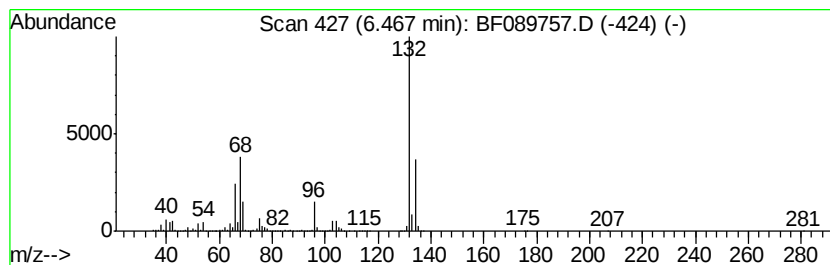
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Peak Number 5 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	65.53 ng	14250900	1,4-Dichlorobenzene-d4	6.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3			Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	12
4			Amphetaminil	250	C17H18N2	017590-01-1	12
5			Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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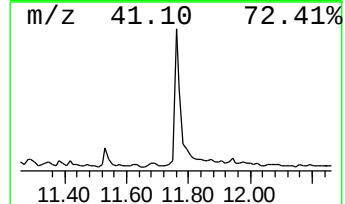
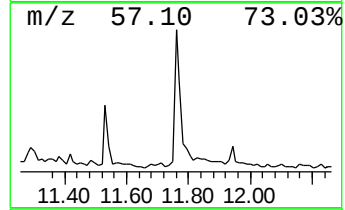
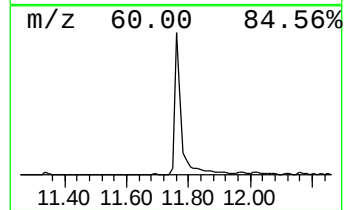
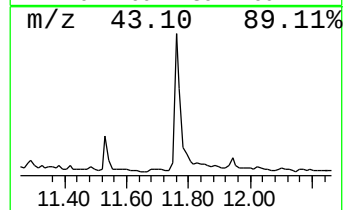
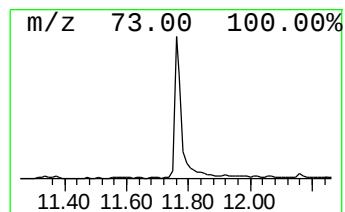
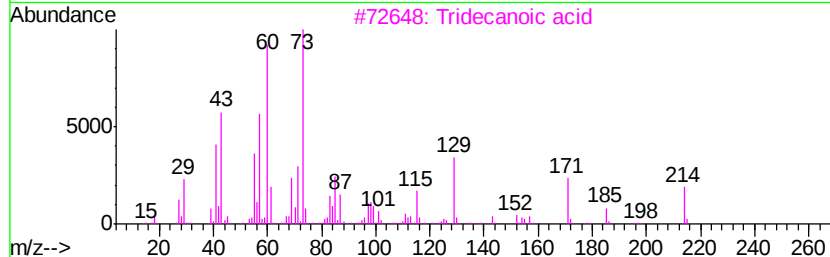
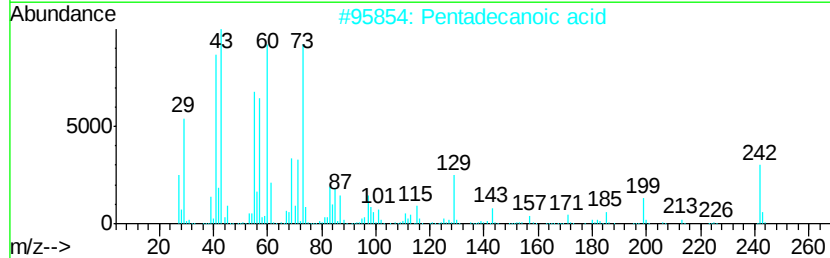
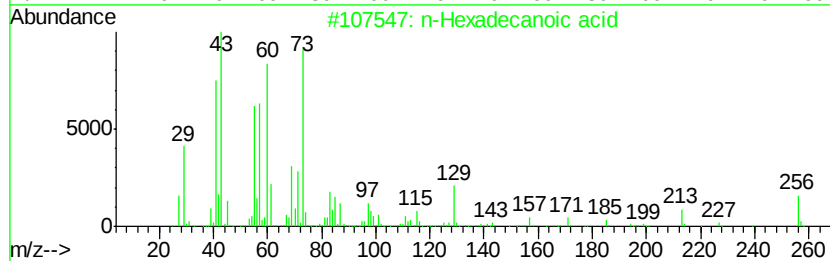
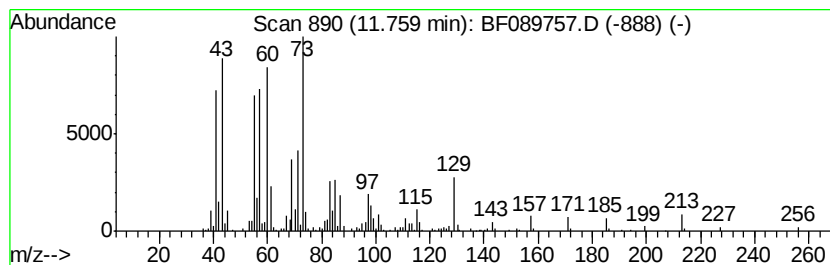
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.82 ng	945671	Phenanthrene-d10	11.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3		Tridecanoic acid	214	C13H26O2	000638-53-9	86
4		Oxalic acid, allvl hexadecyl ester	354	C21H38O4	1000309-24-4	38
5		Oxalic acid, propyl tridecyl ester	314	C18H34O4	1000309-26-6	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.92	17.7	ng	3842160	1	6.70	4349260	20.0
2-Pentanone, 4-hy...	4.86	14.3	ng	3108230	1	6.70	4349260	20.0
unknown6.47	6.47	65.5	ng	14250900	1	6.70	4349260	20.0
n-Hexadecanoic acid	11.76	2.8	ng	945671	4	11.21	6712480	20.0