

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG060817\
 Data File : BG027330.D
 Acq On : 8 Jun 2017 23:35
 Operator : SJ/MA
 Sample : I3479-07
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TW-3-20170603

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-BG060517.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	5.703	336	343	349	rBV	39216	64006	1.52%	0.340%
2	6.138	410	417	429	rVB	433556	766196	18.22%	4.073%
3	7.689	671	681	692	rBV	313481	585712	13.93%	3.114%
4	8.089	740	749	761	rBV	740389	1362719	32.41%	7.245%
5	8.559	822	829	839	rBV	138855	254651	6.06%	1.354%
6	8.882	876	884	896	rBV	540086	1013368	24.10%	5.387%
7	9.716	1017	1026	1034	rBV	513235	1002383	23.84%	5.329%
8	11.373	1301	1308	1315	rBV	230020	434306	10.33%	2.309%
9	13.764	1706	1715	1724	rBV	1674348	2655034	63.14%	14.115%
10	14.569	1845	1852	1859	rBV	63852	97741	2.32%	0.520%
11	15.139	1941	1949	1958	rBV2	395889	699853	16.64%	3.721%
12	16.620	2194	2201	2216	rBV	1512783	2363731	56.21%	12.566%
13	17.889	2407	2417	2429	rBV	543997	919479	21.87%	4.888%
14	18.723	2554	2559	2569	rBV	79458	130996	3.12%	0.696%
15	19.986	2769	2774	2778	rBV3	48120	69727	1.66%	0.371%
16	20.462	2849	2855	2866	rBV	2852487	4204955	100.00%	22.355%
17	21.831	3083	3088	3098	rBV2	60707	107927	2.57%	0.574%
18	22.272	3156	3163	3175	rVB	552258	1047073	24.90%	5.567%
19	22.442	3189	3192	3199	rVB2	24477	42563	1.01%	0.226%
20	25.956	3780	3790	3807	rVB	296354	987663	23.49%	5.251%

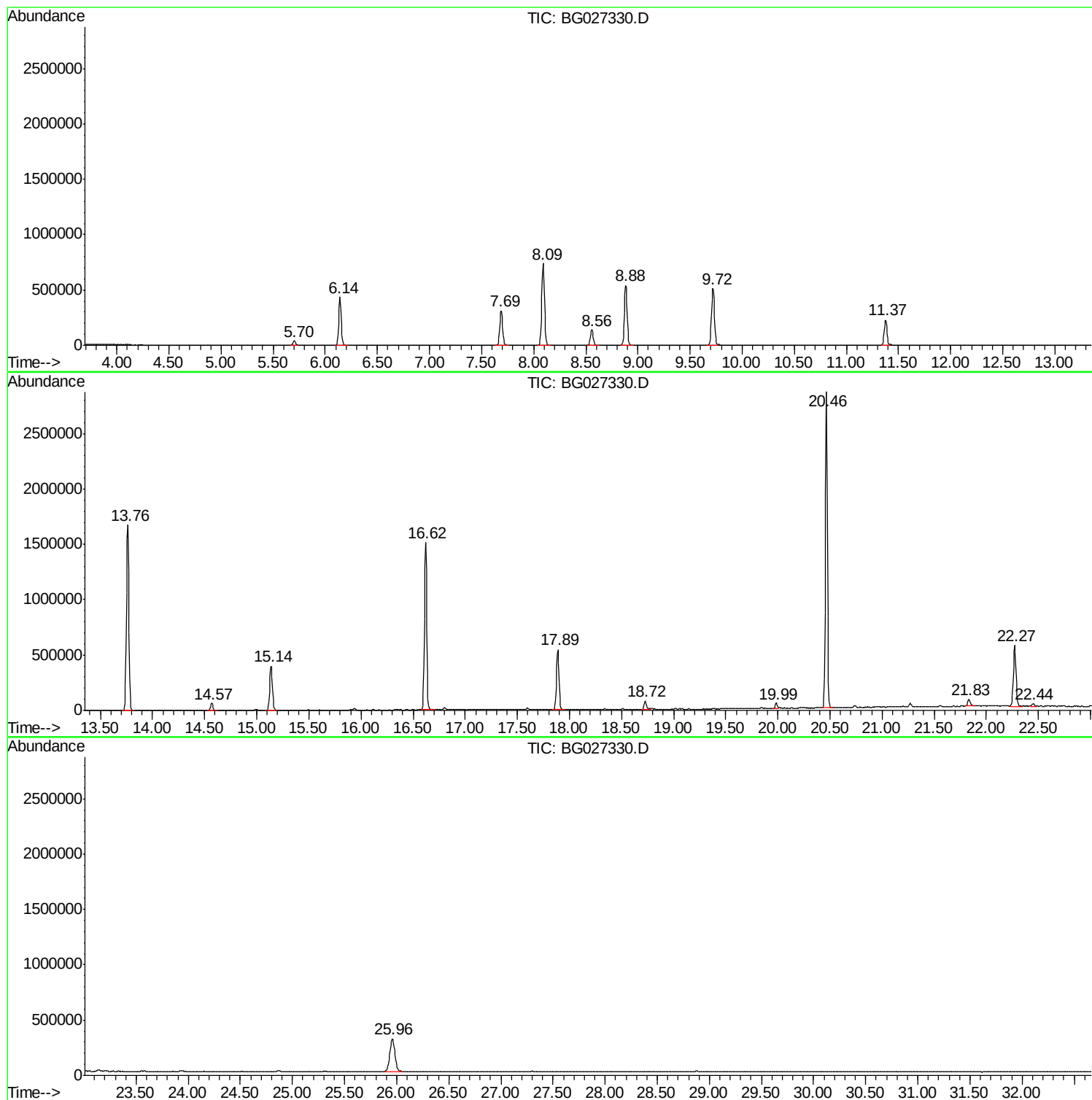
Sum of corrected areas: 18810083

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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060517.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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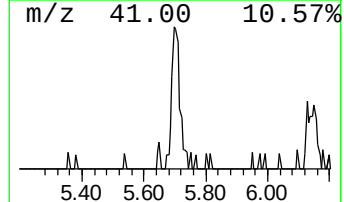
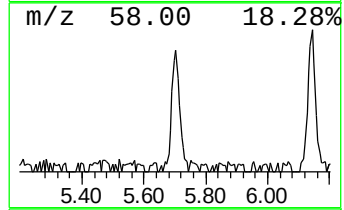
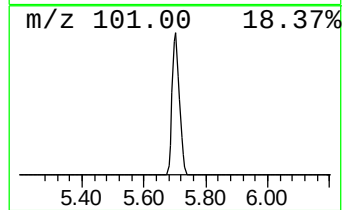
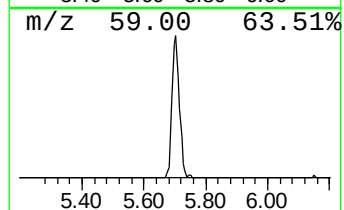
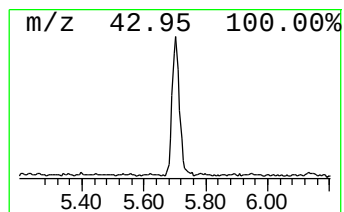
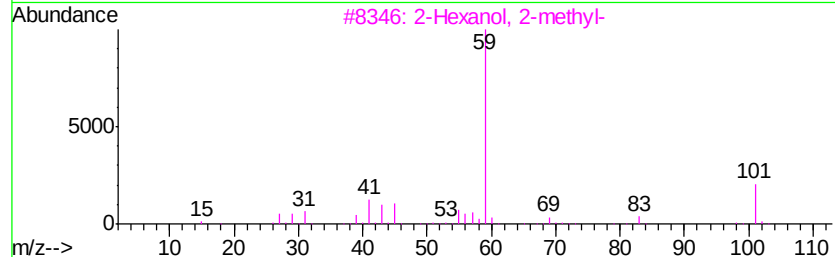
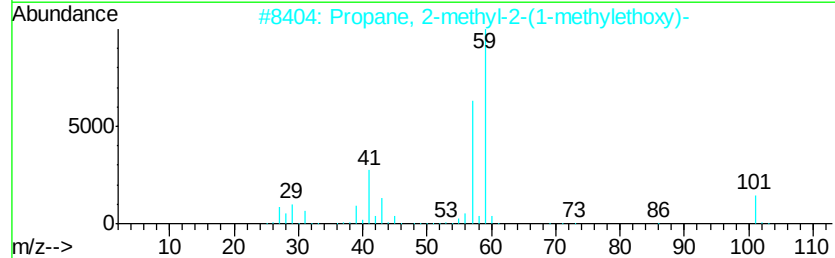
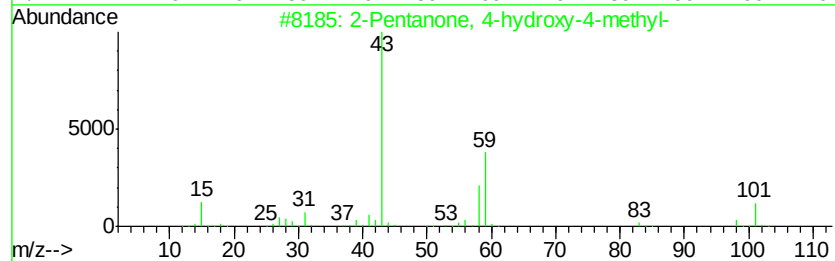
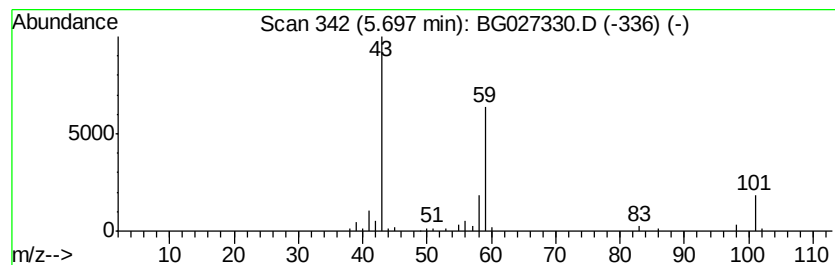
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	5.03 ng	64006	1,4-Dichlorobenzene-d4	8.56

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4		3-Octanol	130	C8H18O	000589-98-0	33
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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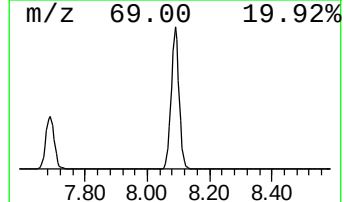
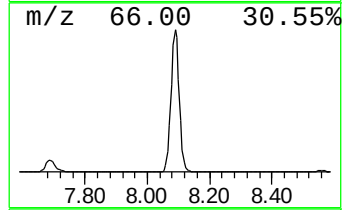
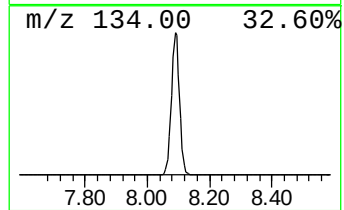
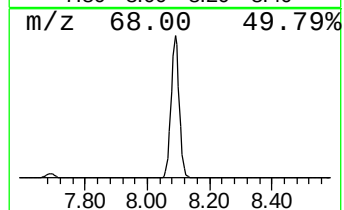
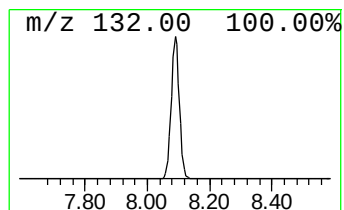
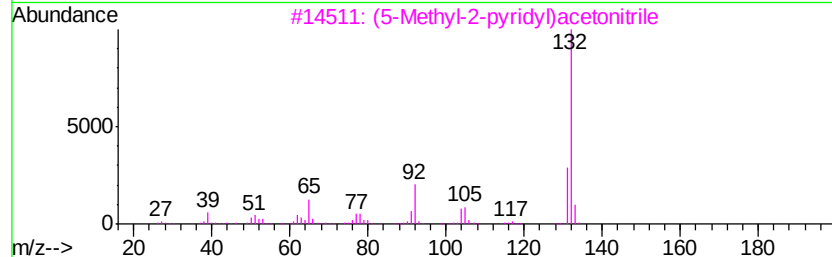
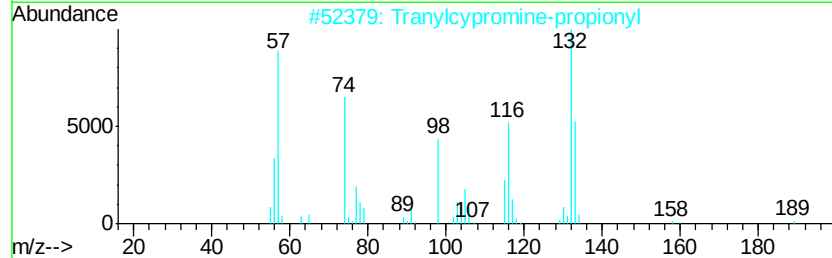
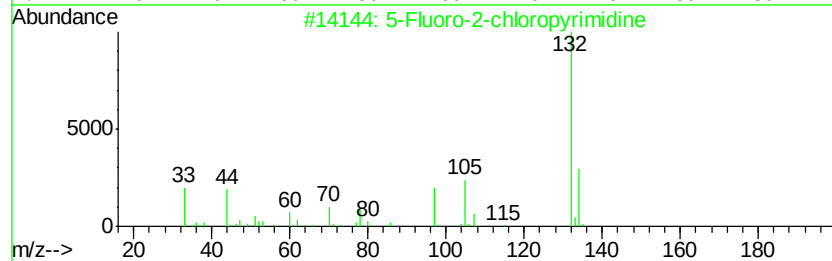
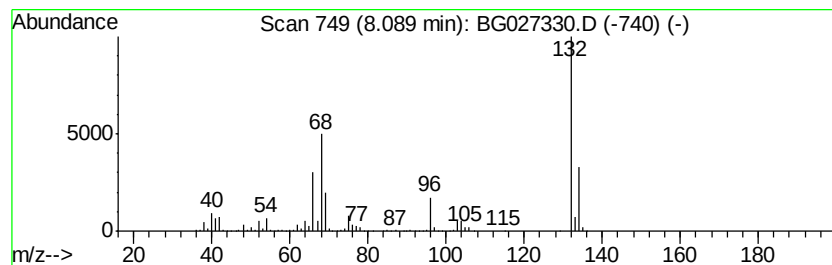
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Peak Number 2 unknown8.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	107.03 ng	1362720	1,4-Dichlorobenzene-d4	8.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Xenon	132	Xe	007440-63-3	9



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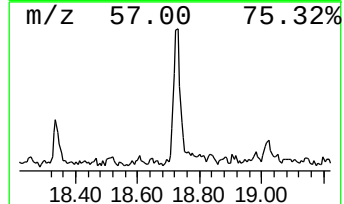
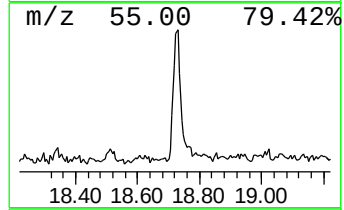
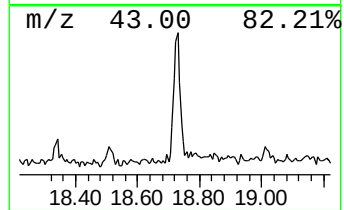
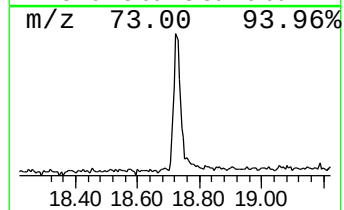
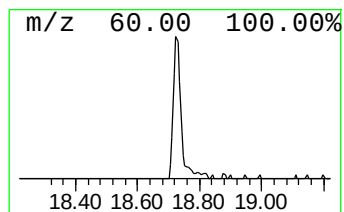
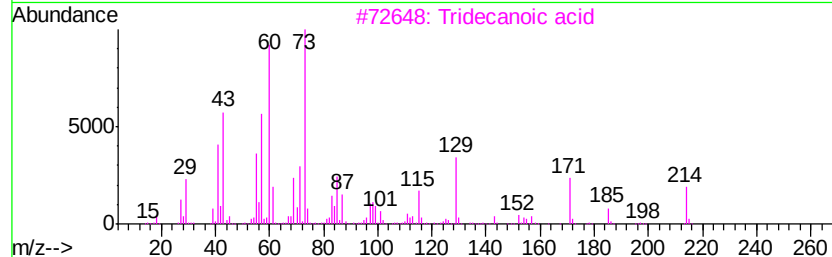
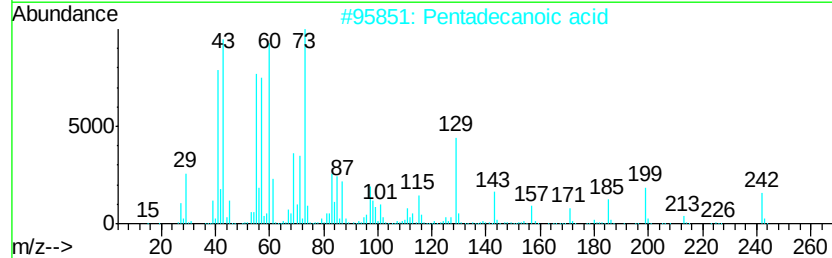
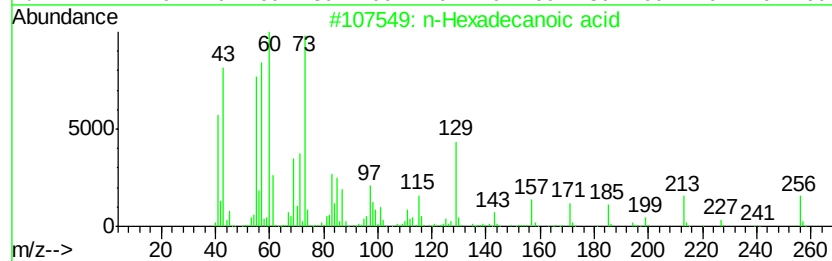
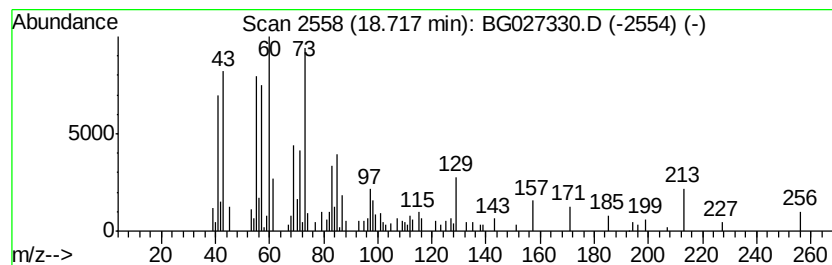
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	2.85 ng	130996	Phenanthrene-d10	17.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5		Isoamyl nitrite	117	C5H11NO2	000110-46-3	22



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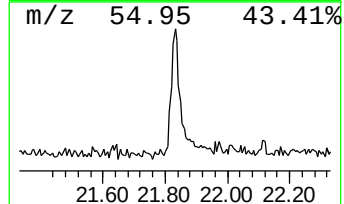
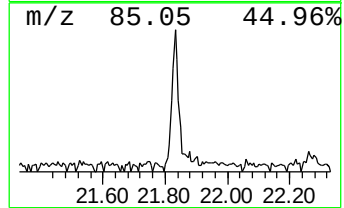
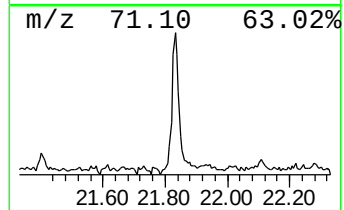
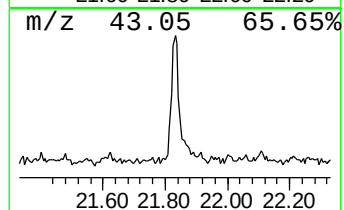
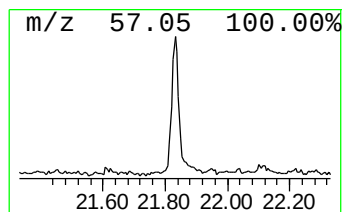
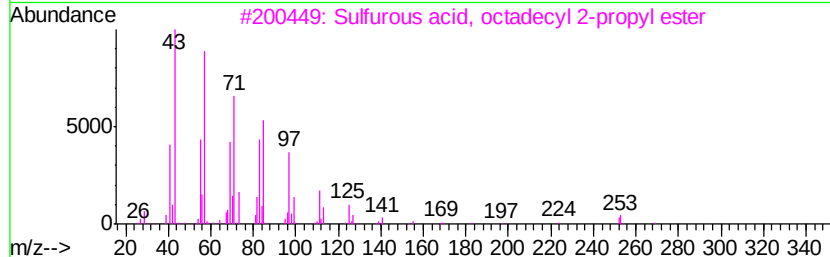
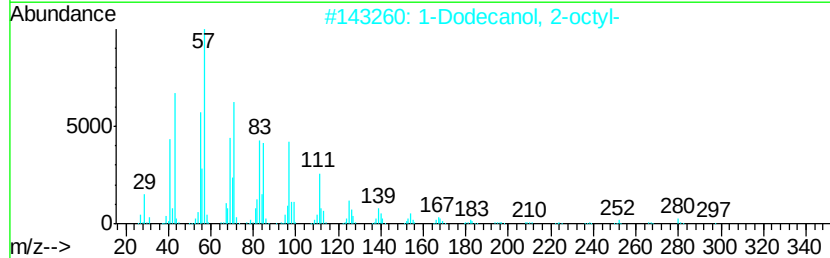
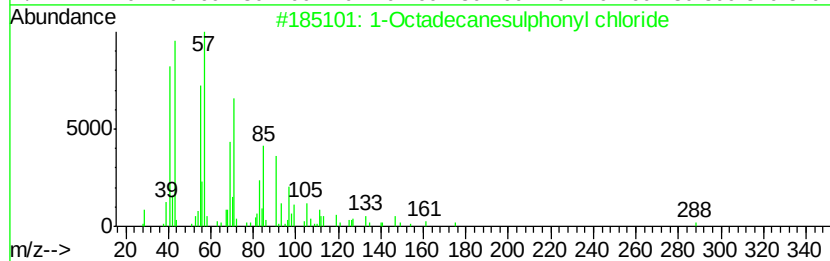
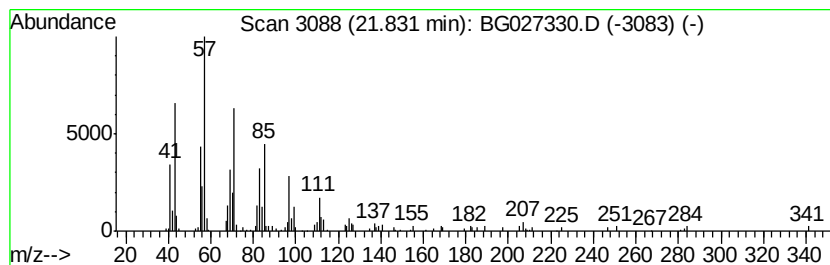
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Peak Number 5 1-Octadecanesulphonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.83	2.06 ng	107927	Chrysene-d12	22.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90
2		1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	86
3		Sulfurous acid, octadecyl 2-propyl-	376	C21H44O3S	1000309-12-7	83
4		Oxalic acid, isobutyl tetradecyl-	342	C20H38O4	1000309-37-9	72
5		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	68



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.70	5.0	ng	64006	1	8.56	254651	20.0
unknown8.09	8.09	107.0	ng	1362720	1	8.56	254651	20.0
n-Hexadecanoic acid	18.72	2.9	ng	130996	4	17.89	919479	20.0
1-Octadecanesulph...	21.83	2.1	ng	107927	5	22.27	1047070	20.0