

Data Path : U:\HPCHEM1\BNA G\DATA\BG010418\
 Data File : BG031926.D
 Acq On : 4 Jan 2018 21:51
 Operator : SJ/JU
 Sample : J1025-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-106-2(75-77)

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-BG122117.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	3.418	17	22	33	rBV	110253	219117	5.34%	1.165%
2	3.506	33	37	45	rVB	25913	42307	1.03%	0.225%
3	5.703	405	411	417	rBV	56099	93853	2.29%	0.499%
4	6.209	489	497	511	rBV	638725	1093184	26.66%	5.810%
5	7.889	774	783	798	rBV	651515	1229040	29.97%	6.532%
6	8.295	844	852	863	rBV	657139	1226018	29.90%	6.516%
7	8.782	929	935	944	rVB	127575	231980	5.66%	1.233%
8	9.123	983	993	1006	rBB	498798	948348	23.13%	5.040%
9	9.981	1130	1139	1154	rBV	359413	692514	16.89%	3.680%
10	11.667	1418	1426	1436	rBV	172809	331274	8.08%	1.761%
11	14.047	1823	1831	1840	rBV	1306602	2140061	52.19%	11.374%
12	14.840	1960	1966	1972	rBV2	125089	197683	4.82%	1.051%
13	15.416	2057	2064	2071	rBV2	338245	560694	13.67%	2.980%
14	16.197	2185	2197	2202	rBV2	27441	43882	1.07%	0.233%
15	16.890	2308	2315	2325	rBV	1389828	2289277	55.83%	12.167%
16	17.055	2338	2343	2354	rVB3	24750	44213	1.08%	0.235%
17	18.148	2522	2529	2540	rBV	553080	868049	21.17%	4.613%
18	18.964	2663	2668	2673	rBV2	79988	115729	2.82%	0.615%
19	20.198	2873	2878	2885	rBV2	52156	81977	2.00%	0.436%
20	20.680	2954	2960	2968	rBV	2902067	4100622	100.00%	21.794%
21	22.031	3185	3190	3197	rBV2	72132	111385	2.72%	0.592%
22	22.490	3261	3268	3278	rVB2	570340	1108921	27.04%	5.894%
23	26.232	3893	3905	3920	rVB2	321311	1045652	25.50%	5.557%

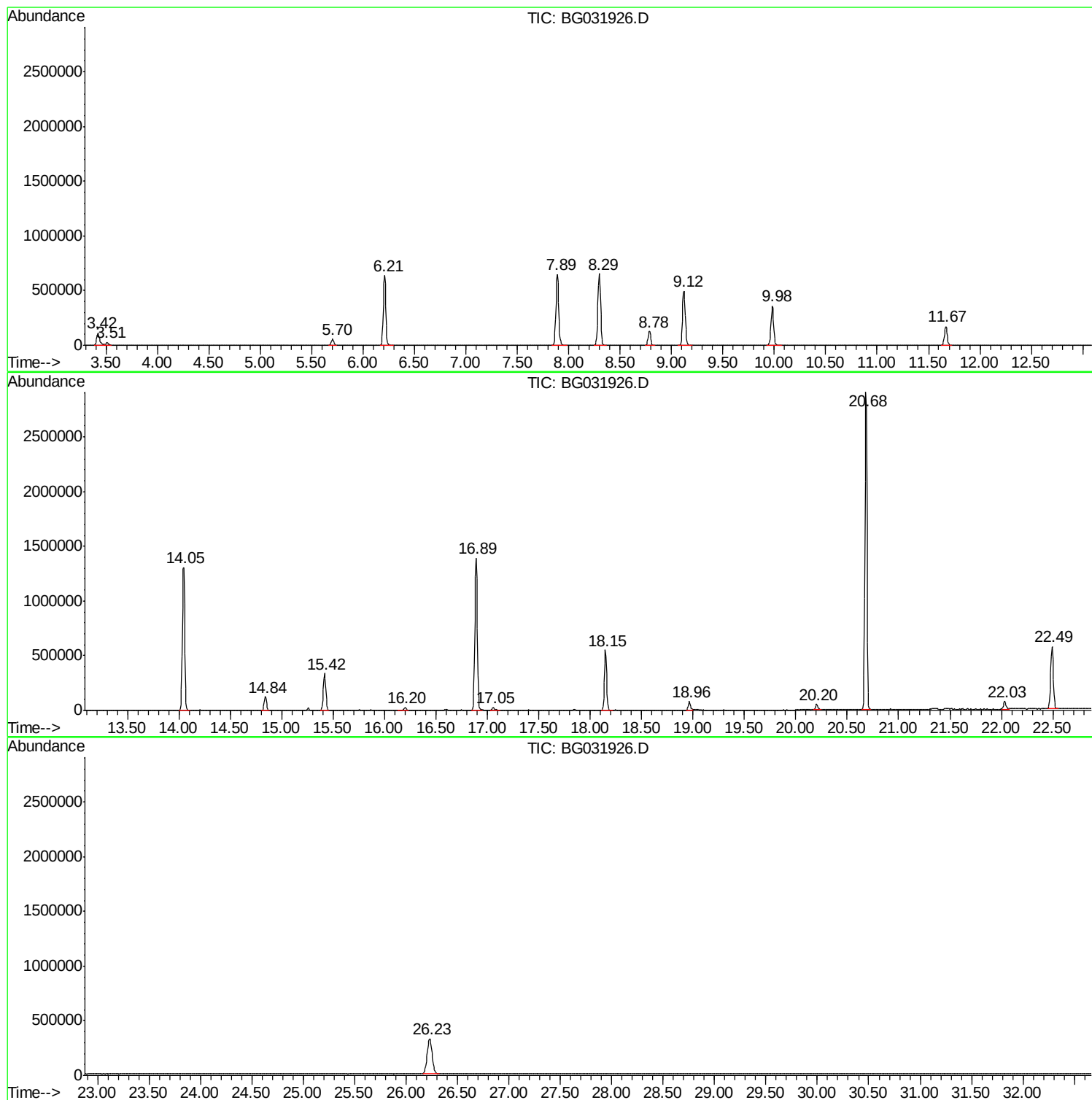
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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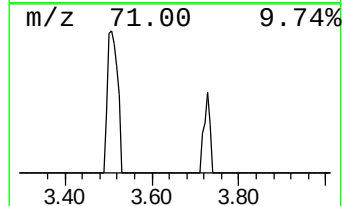
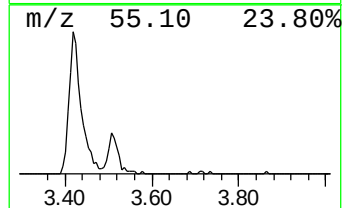
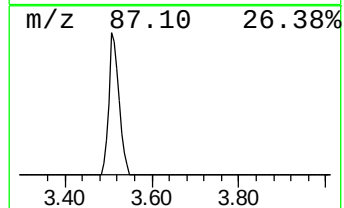
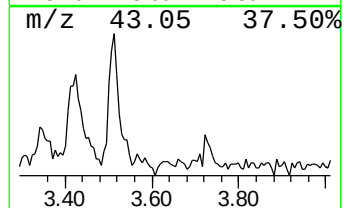
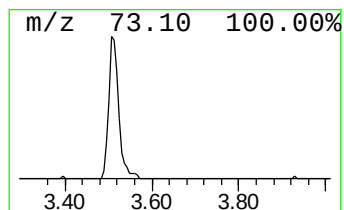
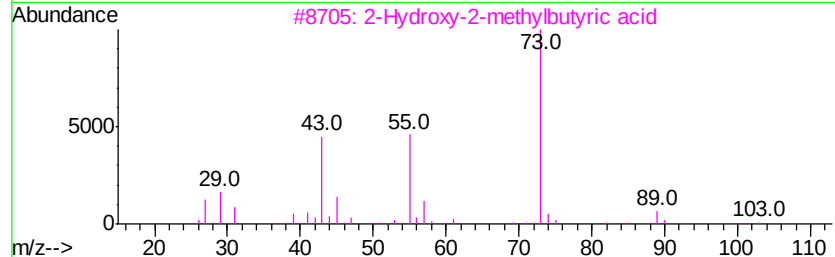
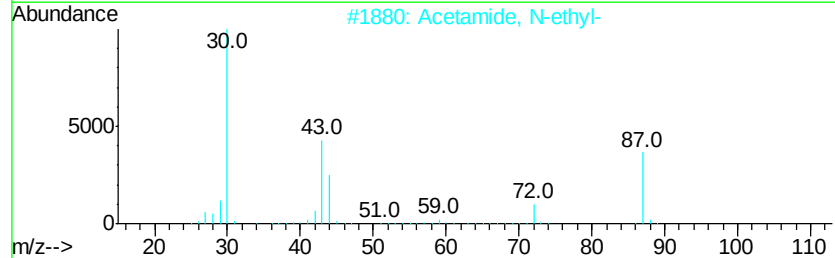
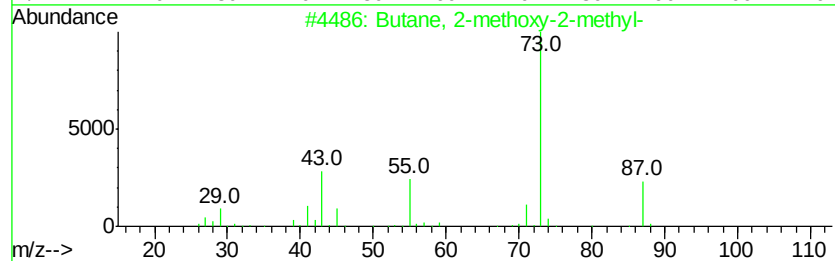
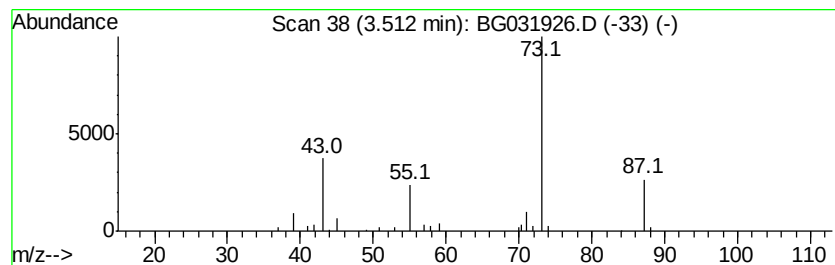
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.51	3.65 ng	42307	1,4-Dichlorobenzene-d4	8.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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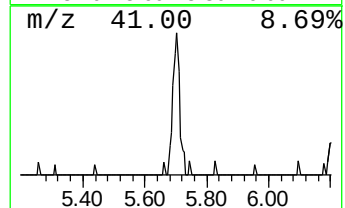
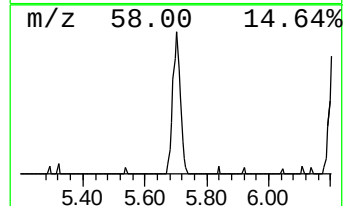
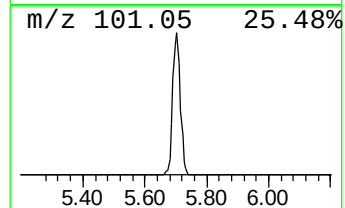
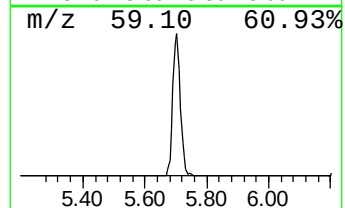
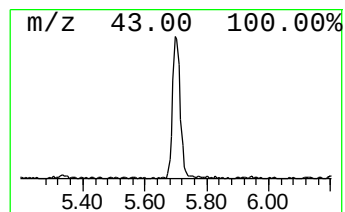
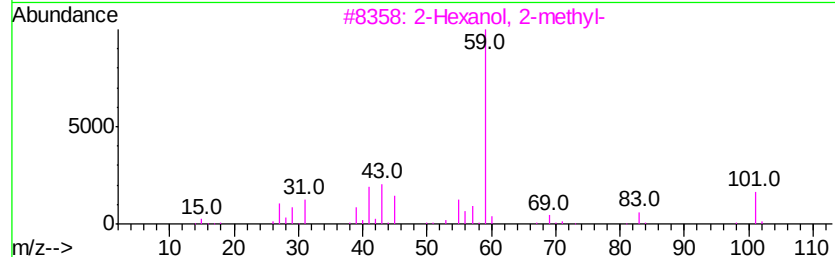
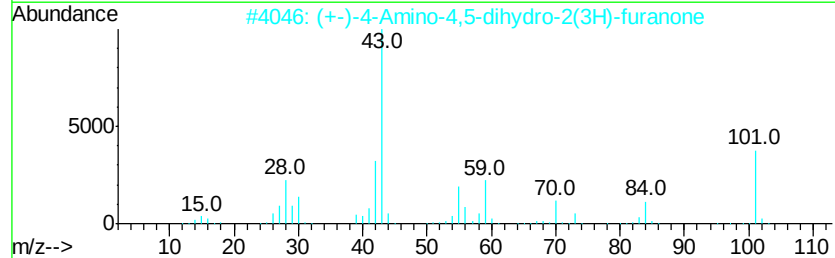
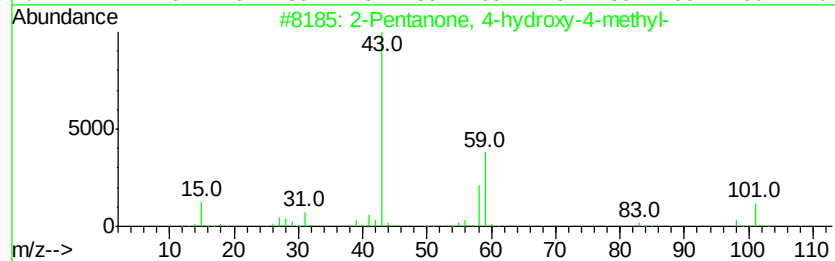
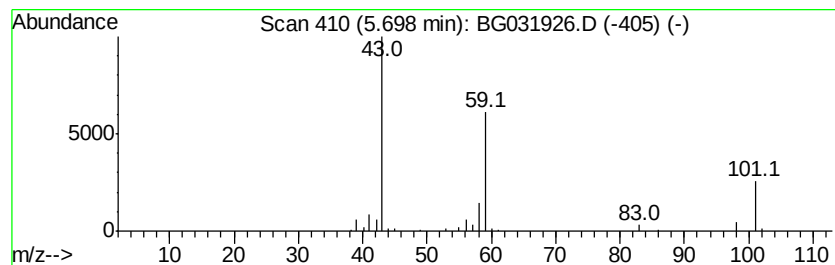
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.70	8.09 ng	93853	1,4-Dichlorobenzene-d4	8.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	37
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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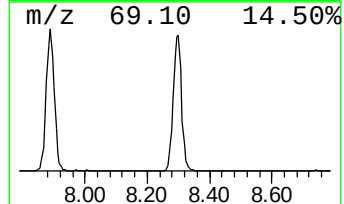
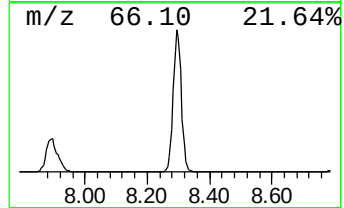
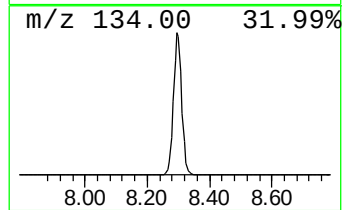
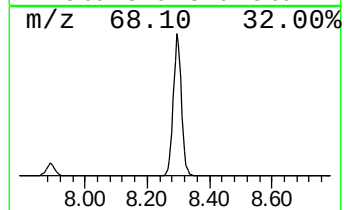
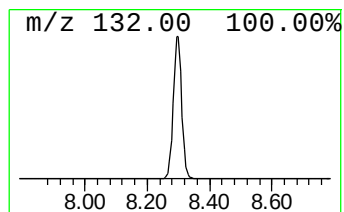
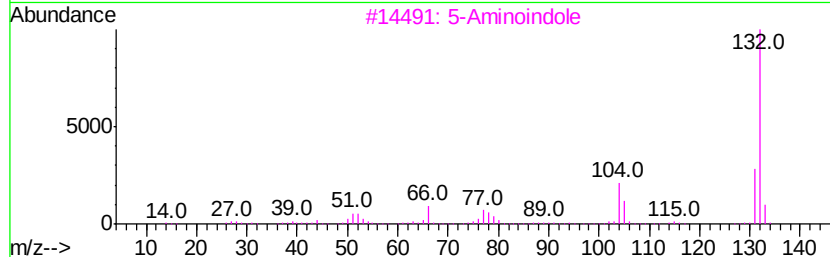
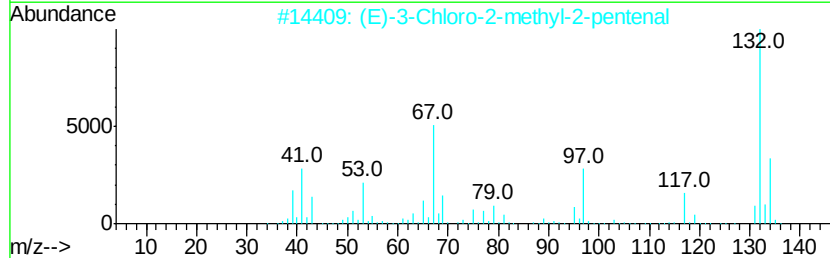
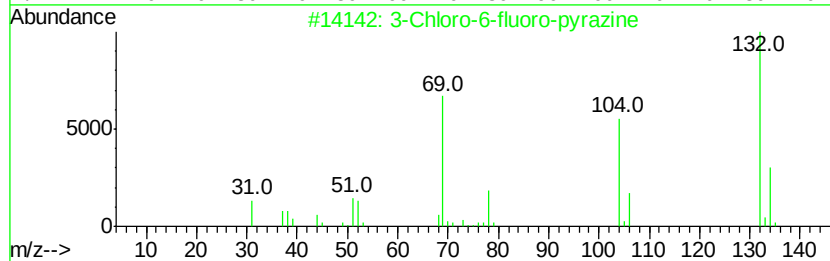
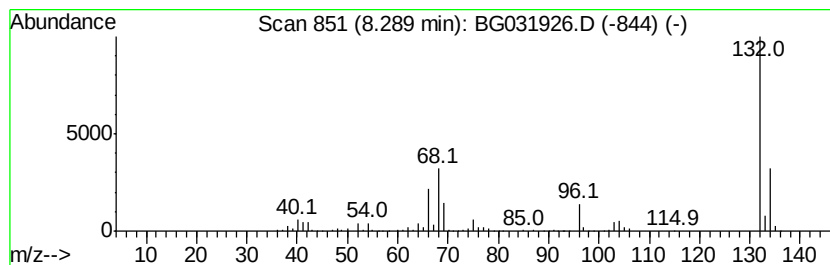
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Peak Number 4 unknown8.29 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	105.70 ng	1226020	1,4-Dichlorobenzene-d4	8.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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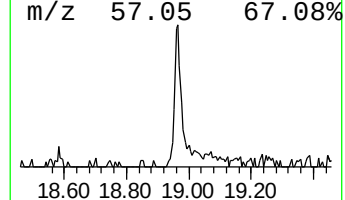
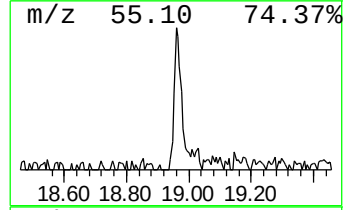
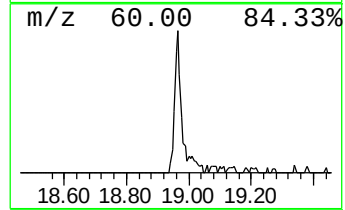
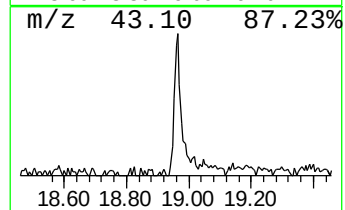
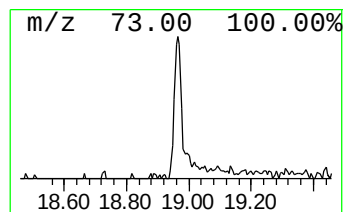
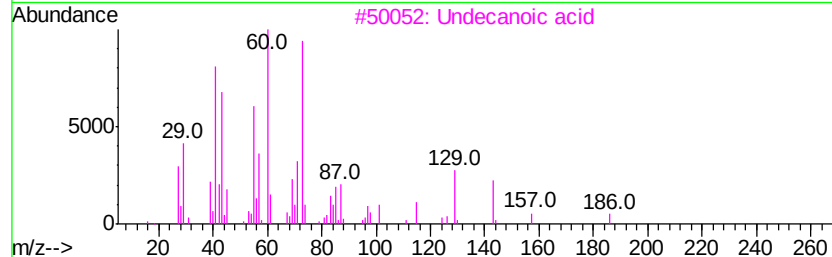
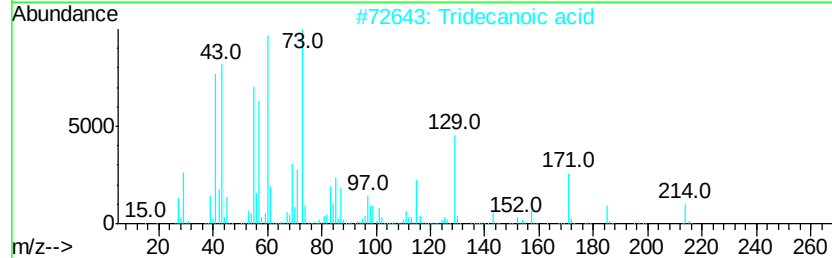
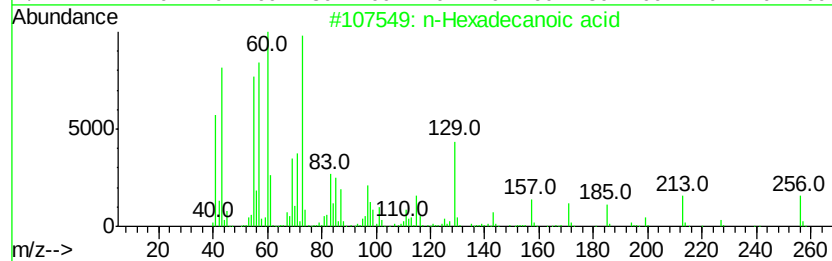
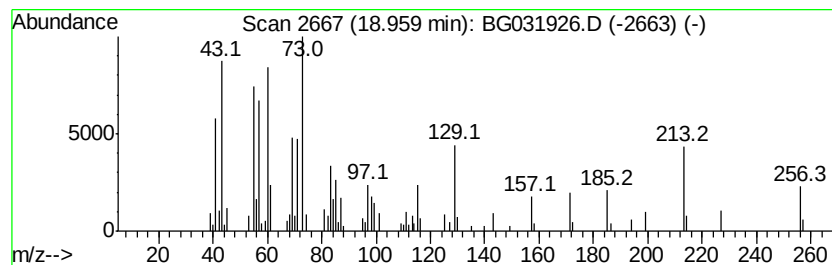
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.96	2.67 ng	115729	Phenanthrene-d10	18.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Undecanoic acid	186	C11H22O2	000112-37-8	55
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	46



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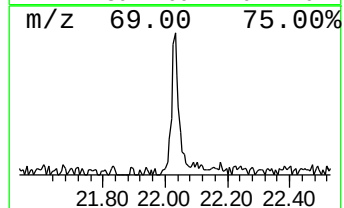
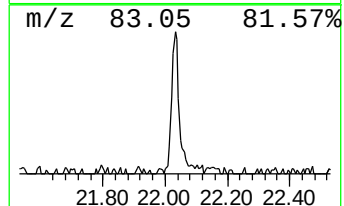
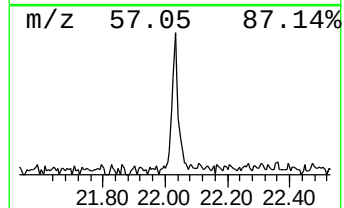
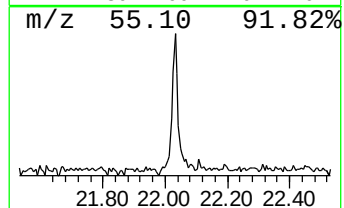
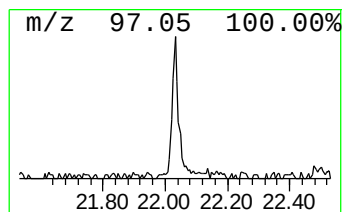
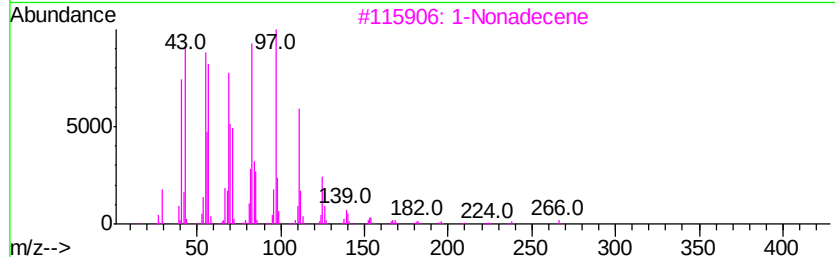
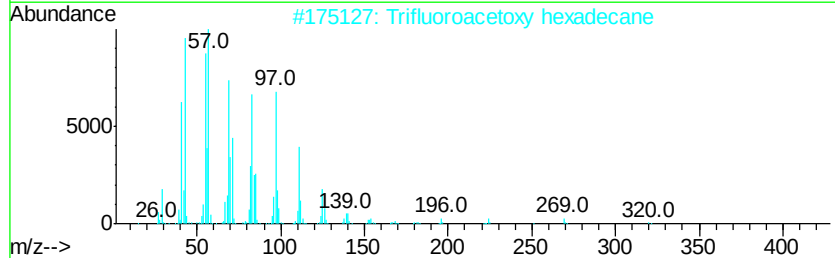
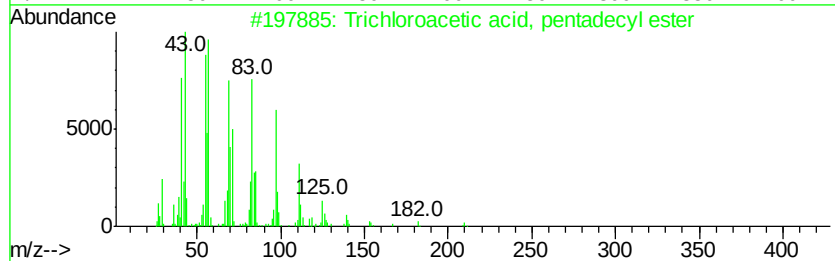
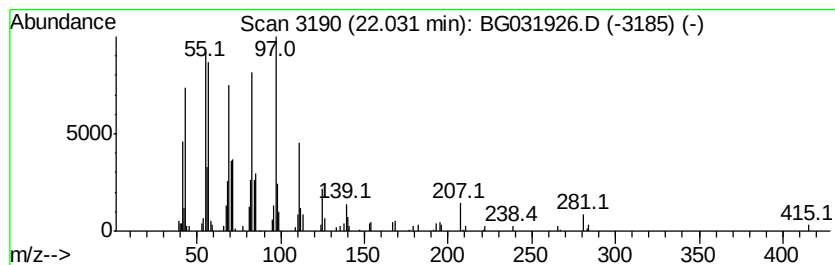
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Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.03	2.01 ng	111385	Chrysene-d12	22.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3		1-Nonadecene	266	C19H38	018435-45-5	81
4		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	76
5		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.51	3.6	ng	42307	1	8.78	231980	20.0
2-Pentanone, 4-hy...	5.70	8.1	ng	93853	1	8.78	231980	20.0
unknown8.29	8.29	105.7	ng	1226020	1	8.78	231980	20.0
n-Hexadecanoic acid	18.96	2.7	ng	115729	4	18.15	868049	20.0
Trichloroacetic a...	22.03	2.0	ng	111385	5	22.49	1108920	20.0