

Data Path : Z:\HPCHEM1\BNA F\DATA\BF050917\
 Data File : BF095045.D
 Acq On : 10 May 2017 3:36
 Operator : SJ/MA
 Sample : I2892-06
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AST-E(9.5-10)

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-BF050217.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	5.031	521	526	543	rBV	180495	357715	12.26%	1.554%
2	5.660	629	633	667	rBV	1432677	2367373	81.11%	10.285%
3	7.260	900	905	920	rBV	1557567	2310335	79.15%	10.037%
4	7.378	920	925	934	rVB	1942034	2600964	89.11%	11.300%
5	7.713	977	982	996	rVB	495566	599218	20.53%	2.603%
6	7.948	1017	1022	1039	rBV	1675582	2025766	69.40%	8.801%
7	8.613	1129	1135	1153	rBV	1003744	1375173	47.11%	5.974%
8	9.731	1320	1325	1346	rBV	618806	809618	27.74%	3.517%
9	11.507	1621	1627	1648	rBV	2287815	2918836	100.00%	12.681%
10	12.201	1739	1745	1756	rBV	208097	302027	10.35%	1.312%
11	12.560	1801	1806	1821	rBV2	615292	931976	31.93%	4.049%
12	13.401	1944	1949	1955	rBV	46203	53051	1.82%	0.230%
13	13.860	2021	2027	2041	rBV	923679	1445078	49.51%	6.278%
14	14.177	2077	2081	2084	rBV	41624	52670	1.80%	0.229%
15	14.966	2210	2215	2219	rBV	525941	733426	25.13%	3.186%
16	15.001	2219	2221	2230	rVB	54026	72181	2.47%	0.314%
17	15.930	2372	2379	2388	rBV5	38645	75225	2.58%	0.327%
18	16.748	2514	2518	2523	rBV	110960	131492	4.50%	0.571%
19	17.048	2566	2569	2578	rVB	120774	144022	4.93%	0.626%
20	17.289	2605	2610	2618	rBV	1647233	1911867	65.50%	8.306%
21	18.542	2818	2823	2833	rBV6	27973	63939	2.19%	0.278%
22	18.630	2833	2838	2842	rBV	517390	655768	22.47%	2.849%
23	19.759	3025	3030	3034	rVB	75260	87599	3.00%	0.381%
24	19.901	3049	3054	3057	rBV	81018	122955	4.21%	0.534%
25	19.924	3057	3058	3063	rVB2	39215	38011	1.30%	0.165%
26	20.189	3099	3103	3106	rBV	50759	62750	2.15%	0.273%
27	20.248	3110	3113	3117	rVV	68647	76596	2.62%	0.333%
28	20.295	3117	3121	3132	rVV2	427945	595843	20.41%	2.589%
29	21.606	3340	3344	3350	rBV2	30864	58689	2.01%	0.255%
30	21.994	3405	3410	3416	rVB3	17764	37484	1.28%	0.163%

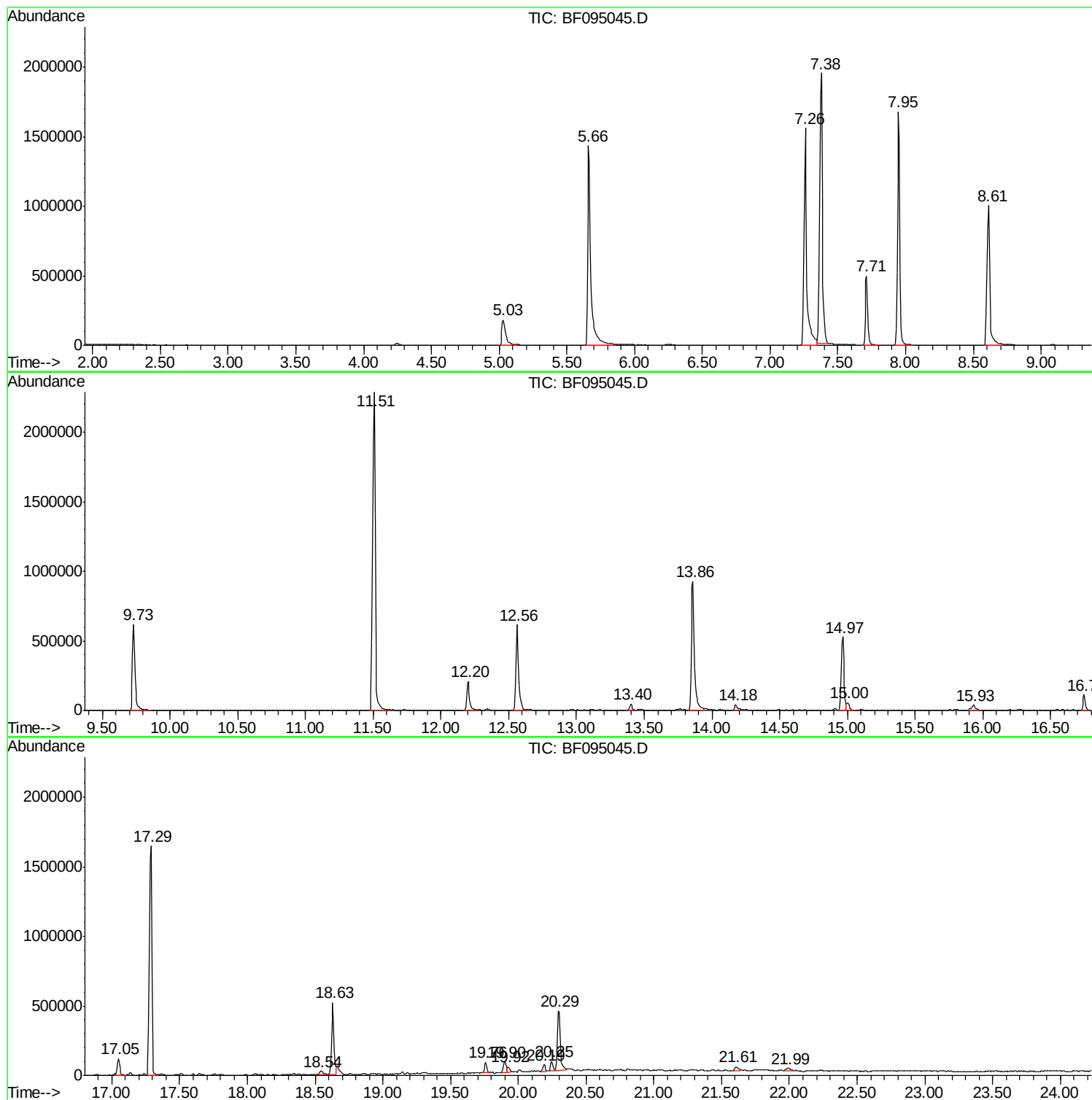
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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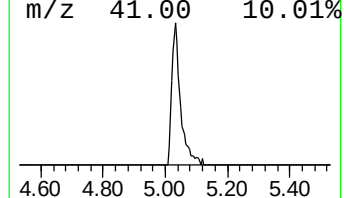
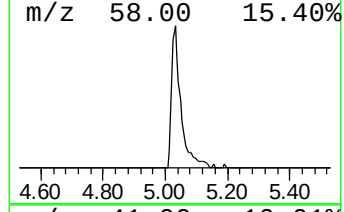
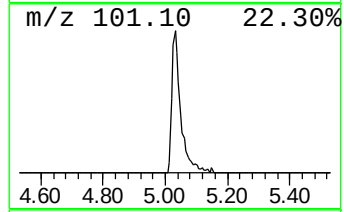
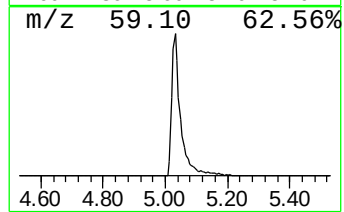
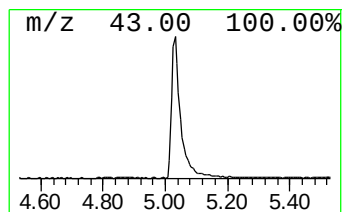
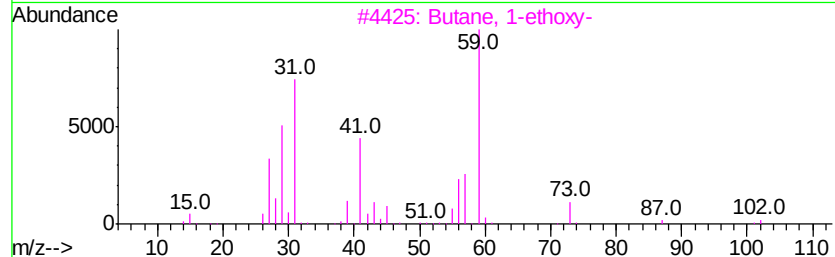
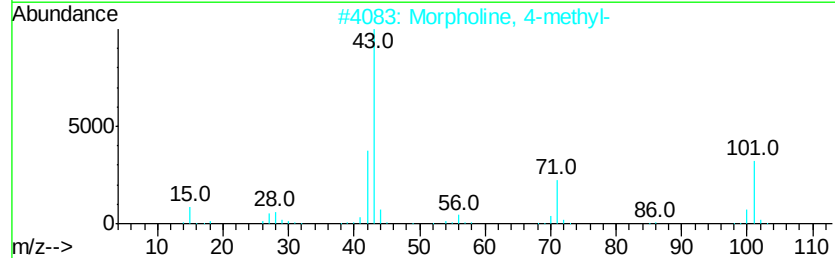
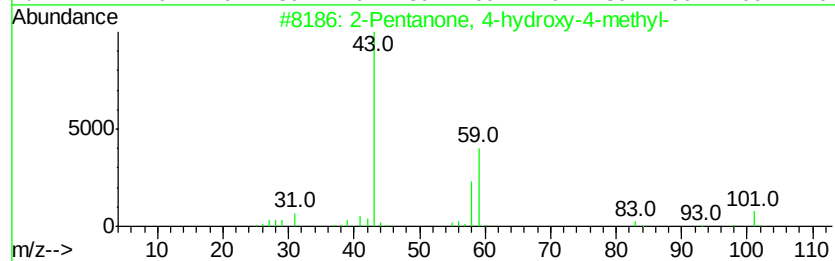
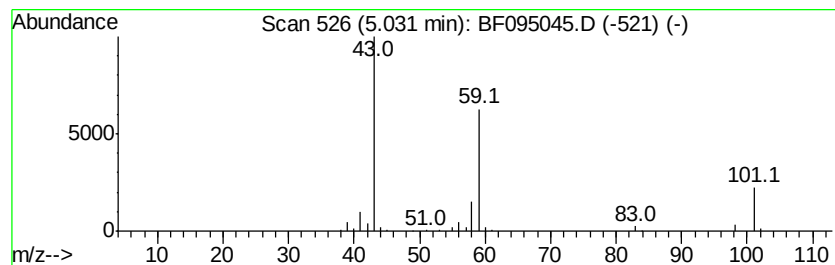
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.03	11.94 ng	357715	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	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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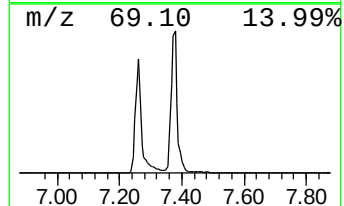
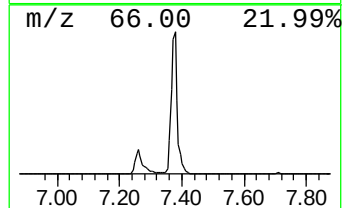
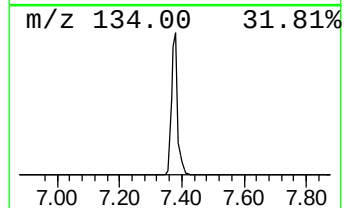
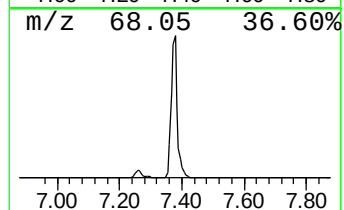
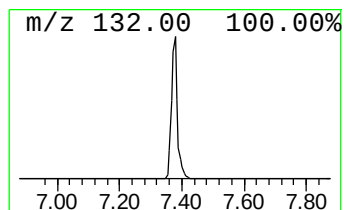
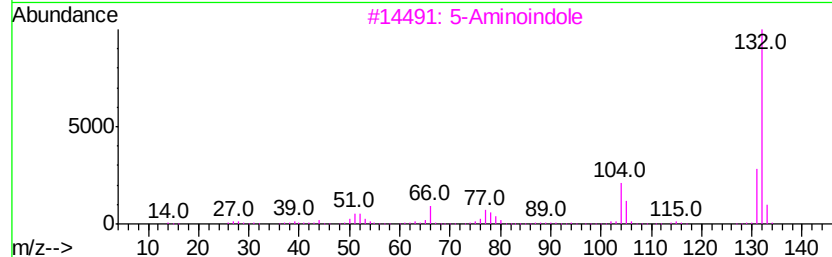
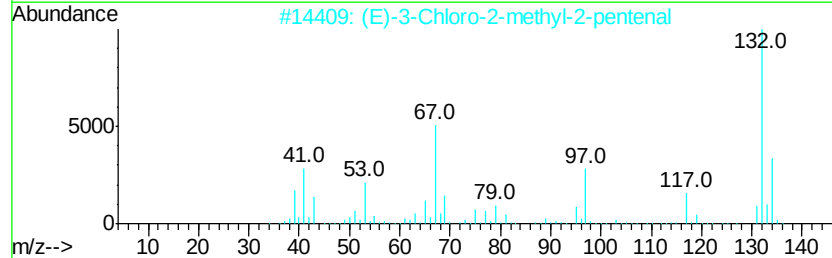
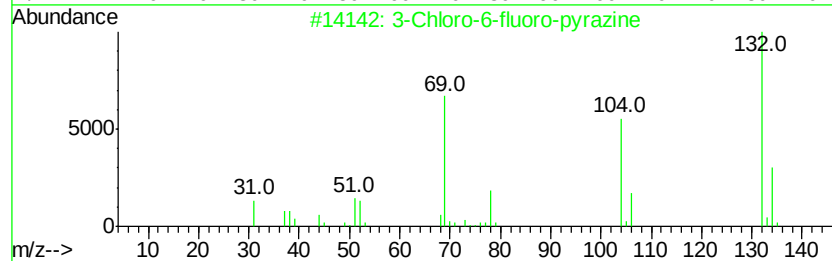
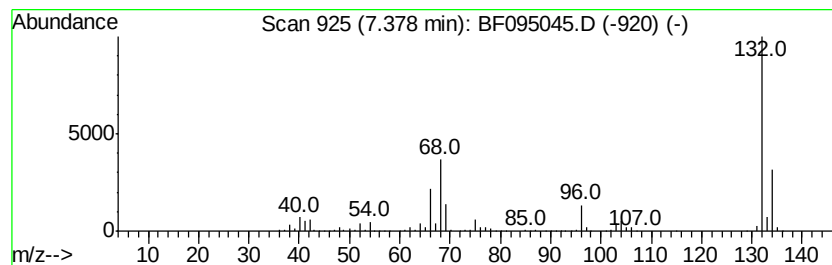
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	86.81 ng	2600960	1,4-Dichlorobenzene-d4	7.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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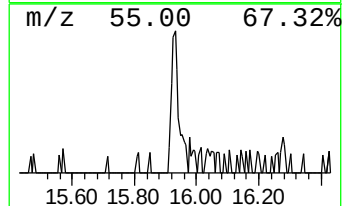
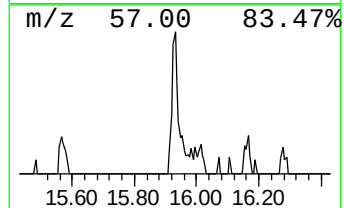
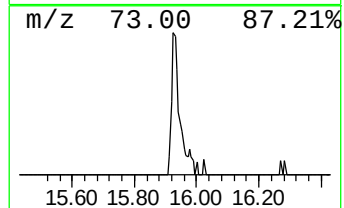
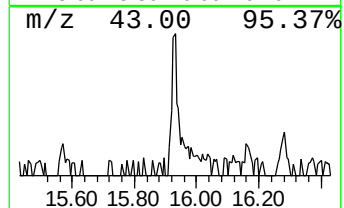
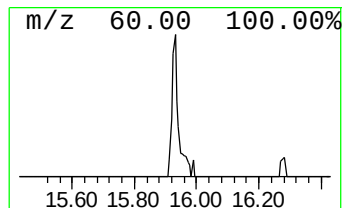
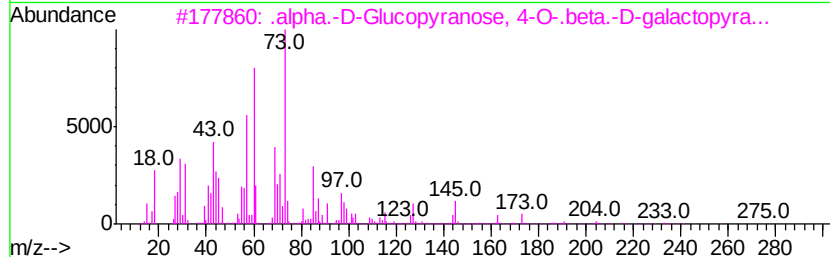
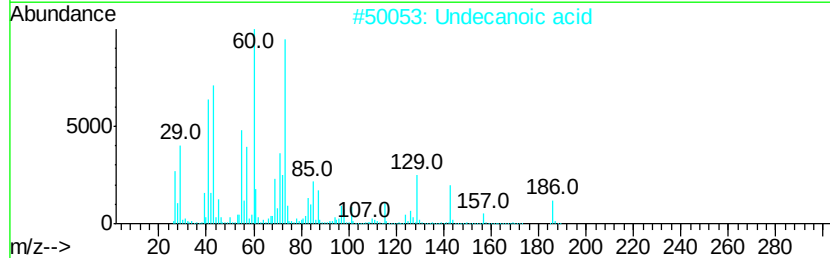
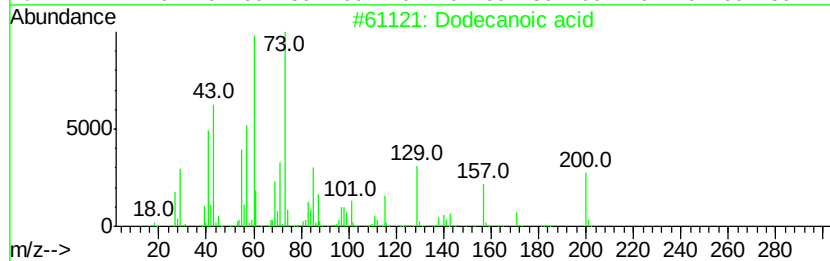
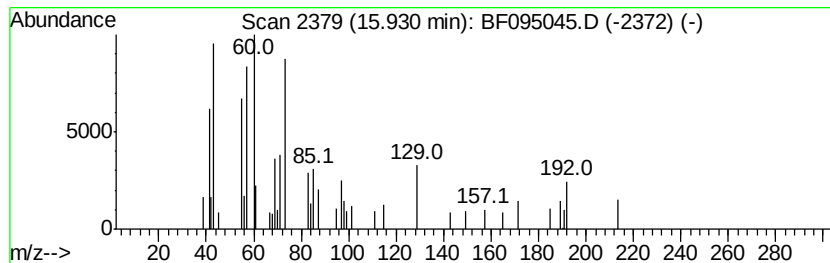
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Peak Number 4 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	2.05 ng	75225	Phenanthrene-d10	14.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	64
2			Undecanoic acid	186	C11H22O2	000112-37-8	59
3			.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	50
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Nonanoic acid	158	C9H18O2	000112-05-0	47



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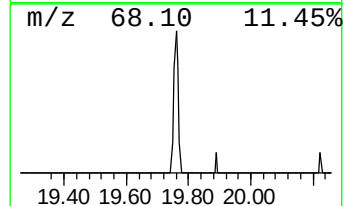
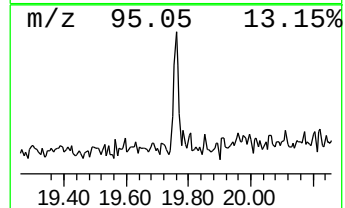
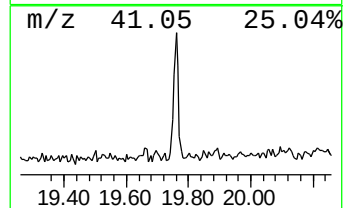
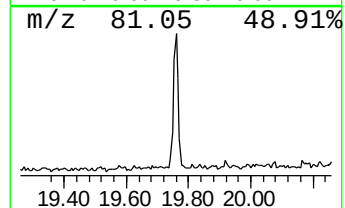
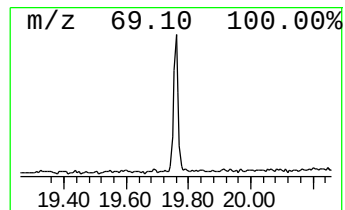
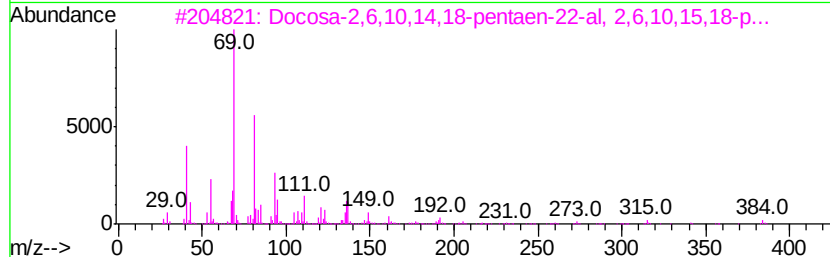
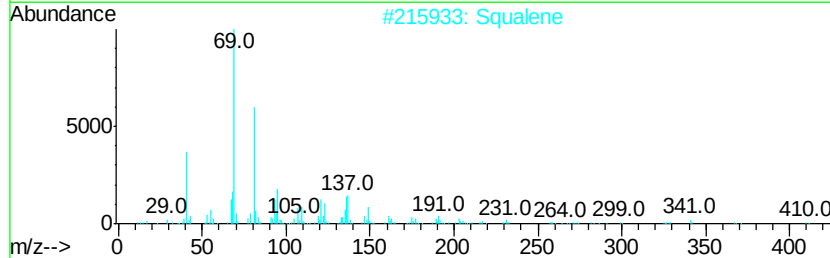
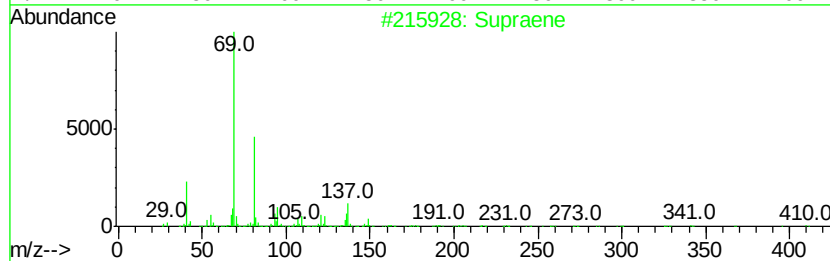
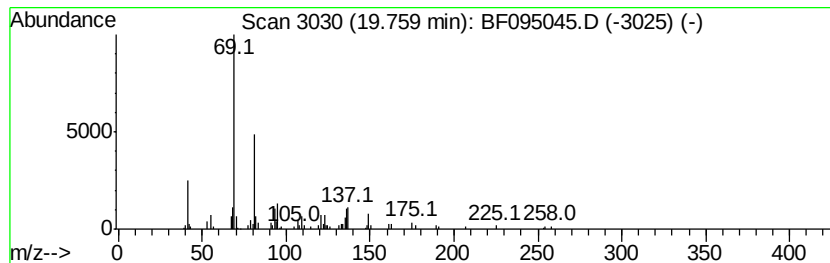
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Peak Number 5 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.76	2.94 ng	87599	Perylene-d12	20.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	90
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	Farnesol (E), methyl ether	236	C16H28O	1000352-67-3	72
5	4,8,12-Tetradecatrilal, 5,9,13-...	248	C17H28O	066408-55-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.03	11.9	ng	357715	1	7.71	599218	20.0
unknown7.38	7.38	86.8	ng	2600960	1	7.71	599218	20.0
Dodecanoic acid	15.93	2.0	ng	75225	4	14.97	733426	20.0
Supraene	19.76	2.9	ng	87599	6	20.30	595843	20.0