

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050417\
 Data File : BF094886.D
 Acq On : 4 May 2017 21:43
 Operator : SJ/MA
 Sample : I2956-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CHERRY-ST-TP(0-5)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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	5.019	520	524	538	rBV	153112	284293	15.03%	1.626%
2	5.666	630	634	661	rBV	1038811	1575100	83.30%	9.011%
3	7.260	900	905	921	rBV	1187075	1576216	83.36%	9.017%
4	7.378	921	925	943	rVB	1288073	1737502	91.89%	9.940%
5	7.719	979	983	992	rBV	379127	425172	22.48%	2.432%
6	7.954	1019	1023	1033	rBV	1048195	1270853	67.21%	7.270%
7	8.613	1130	1135	1154	rBV	761306	990822	52.40%	5.668%
8	9.742	1322	1327	1339	rBV	458162	581912	30.77%	3.329%
9	11.513	1623	1628	1647	rBV	1500631	1756452	92.89%	10.048%
10	12.207	1741	1746	1753	rBV	224416	274738	14.53%	1.572%
11	12.571	1803	1808	1820	rBV2	495767	681386	36.03%	3.898%
12	13.342	1934	1939	1945	rBV3	14155	20170	1.07%	0.115%
13	13.413	1948	1951	1957	rVB	46589	51268	2.71%	0.293%
14	13.777	2005	2013	2016	rBV3	15878	30245	1.60%	0.173%
15	13.860	2022	2027	2043	rBV	809541	1134585	60.00%	6.491%
16	14.189	2078	2083	2085	rBV	56504	67013	3.54%	0.383%
17	14.207	2085	2086	2092	rVB2	22170	27077	1.43%	0.155%
18	14.918	2203	2207	2211	rBV	45322	51468	2.72%	0.294%
19	14.971	2211	2216	2220	rVV	542484	706415	37.36%	4.041%
20	15.007	2220	2222	2227	rVB	49928	58608	3.10%	0.335%
21	15.577	2315	2319	2324	rVB	24902	28573	1.51%	0.163%
22	15.936	2376	2380	2389	rVB2	108799	134243	7.10%	0.768%
23	16.754	2515	2519	2525	rBV	94047	107045	5.66%	0.612%
24	17.054	2566	2570	2575	rVB	115716	133984	7.09%	0.767%
25	17.295	2606	2611	2615	rBV	1717409	1890931	100.00%	10.818%
26	17.648	2668	2671	2676	rBV3	13481	21311	1.13%	0.122%
27	18.548	2818	2824	2833	rBV2	87326	191276	10.12%	1.094%
28	18.630	2833	2838	2843	rBV	631024	768190	40.62%	4.395%
29	19.771	3029	3032	3036	rVB	85885	81872	4.33%	0.468%
30	19.900	3050	3054	3057	rBV	44848	69067	3.65%	0.395%
31	20.189	3099	3103	3109	rVB	37741	42599	2.25%	0.244%
32	20.242	3109	3112	3117	rBV	38415	45481	2.41%	0.260%
33	20.294	3117	3121	3136	rVV	453887	595736	31.50%	3.408%
34	21.600	3339	3343	3348	rBV3	18171	34336	1.82%	0.196%

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ClientSampleId :
CHERRY-ST-TP(0-5)

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

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35	21.977	3402	3407	3414	rVB2	17857	33926	1.79%	0.194%
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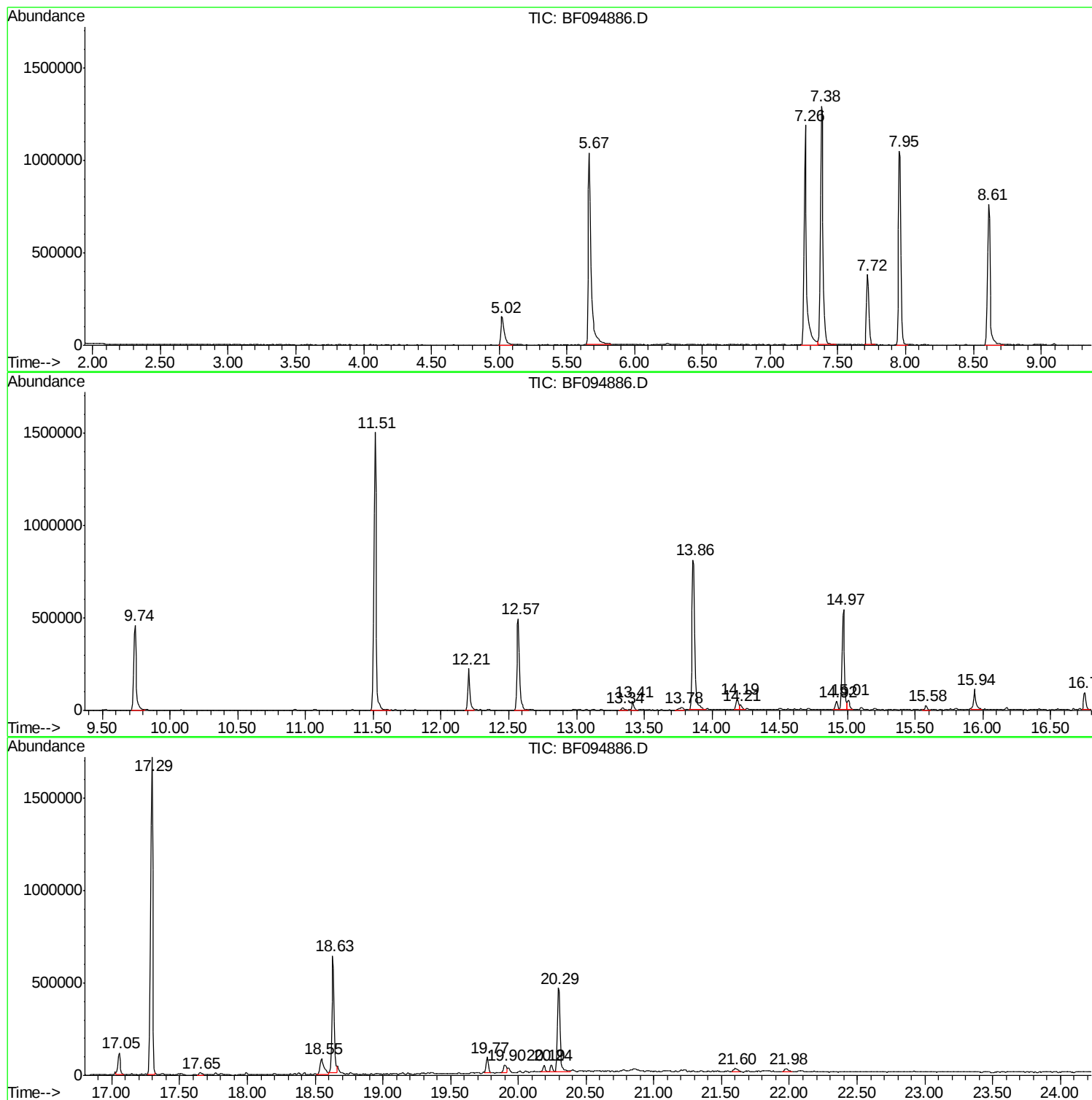
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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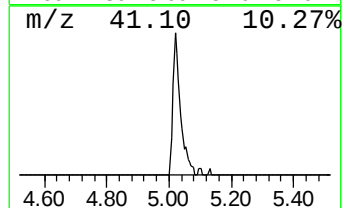
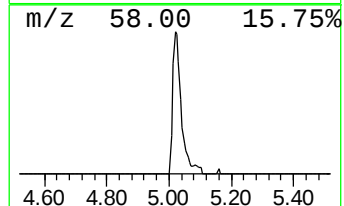
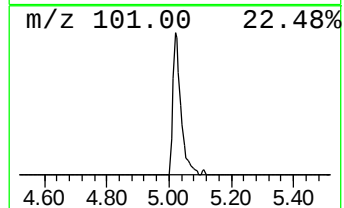
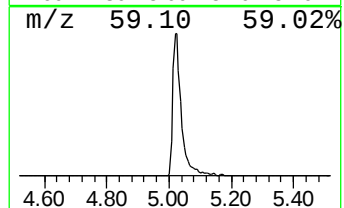
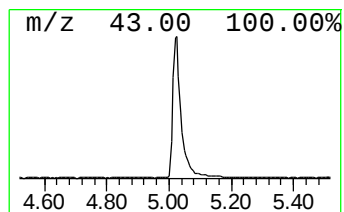
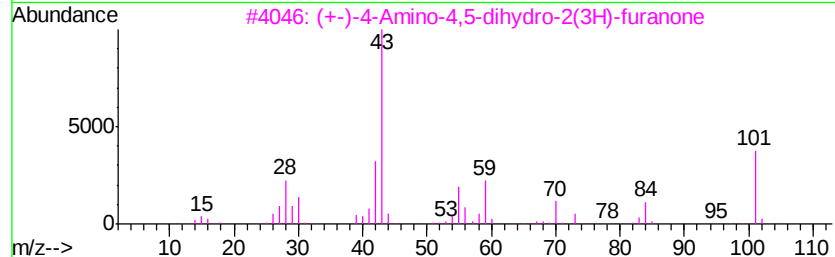
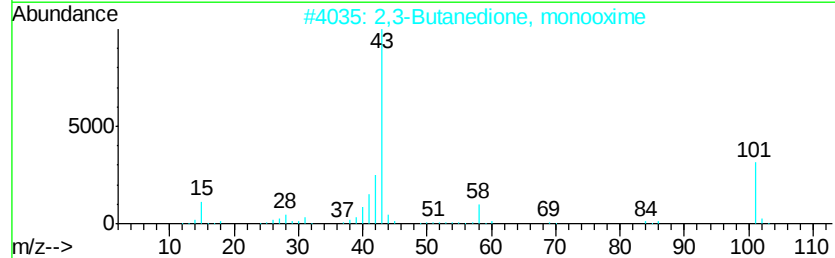
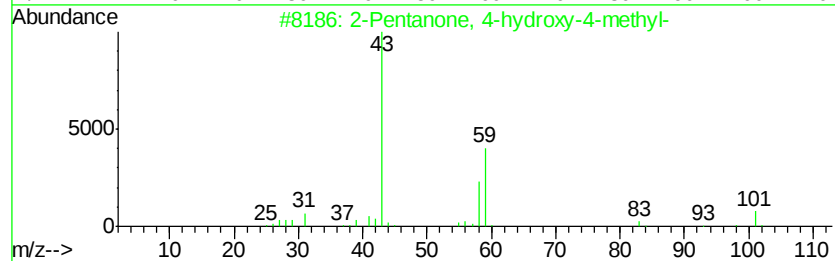
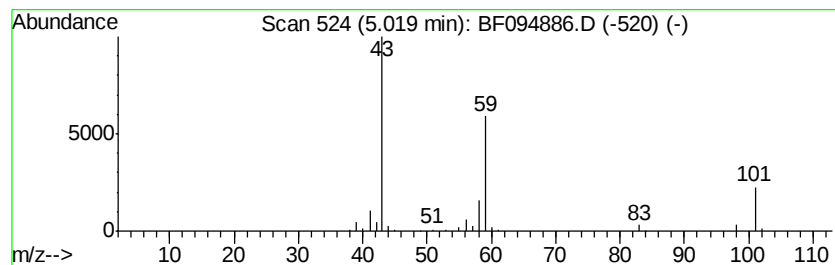
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.02	13.37 ng	284293	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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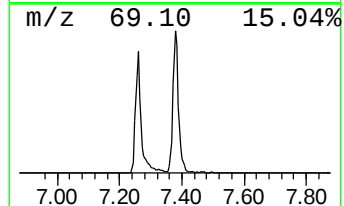
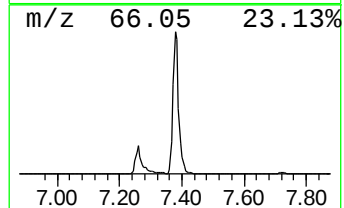
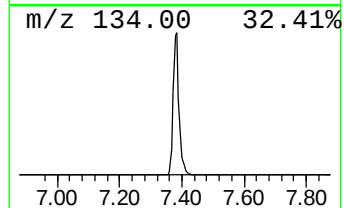
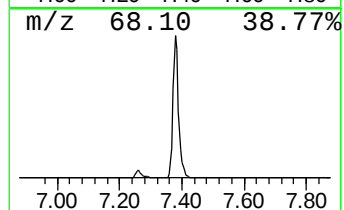
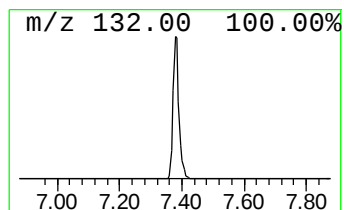
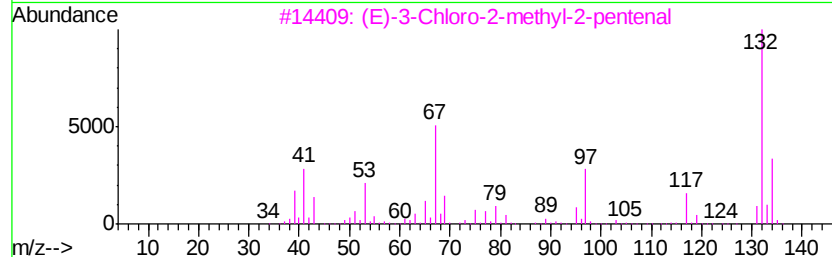
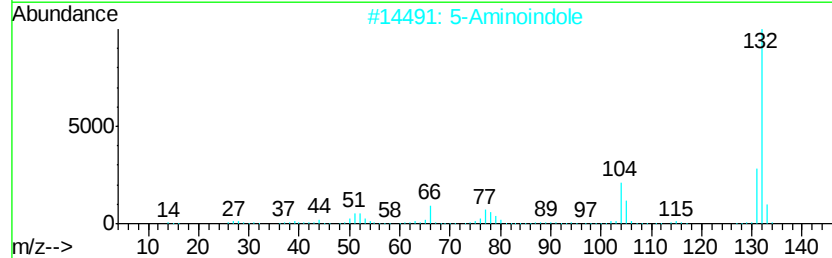
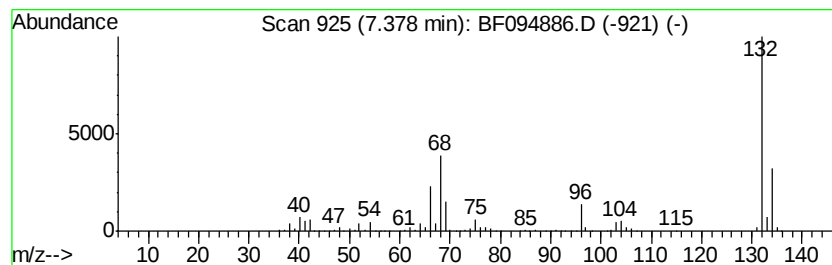
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Peak Number 2 unknown7.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	81.73 ng	1737500	1,4-Dichlorobenzene-d4	7.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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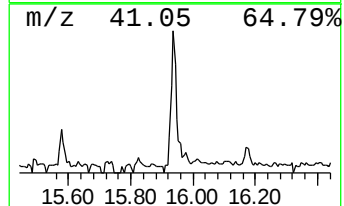
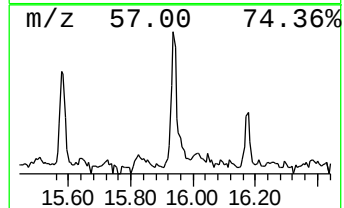
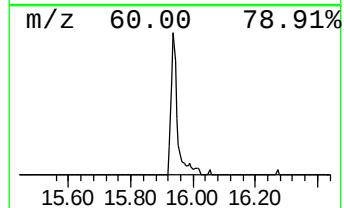
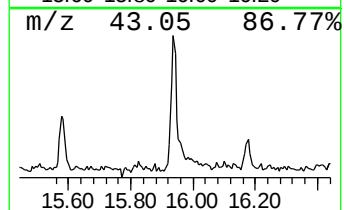
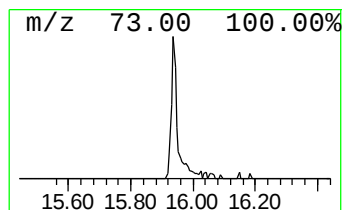
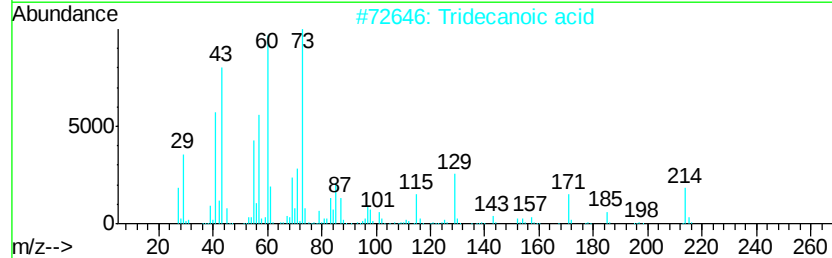
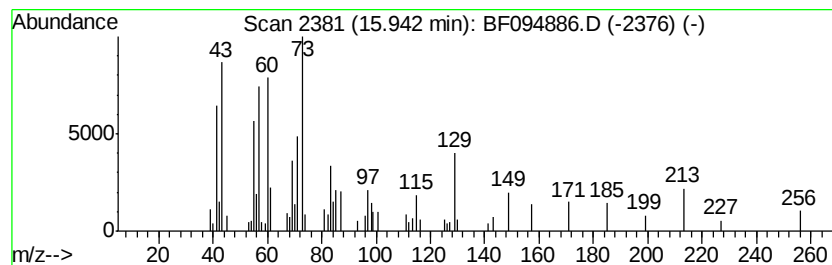
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	3.80 ng	134243	Phenanthrene-d10	14.97

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	90
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5		Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18



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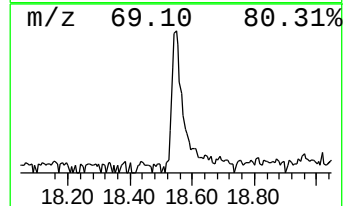
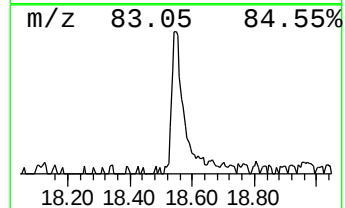
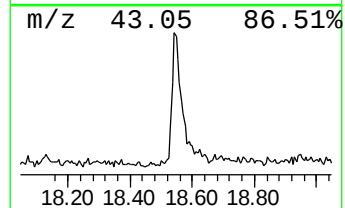
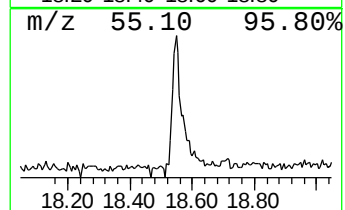
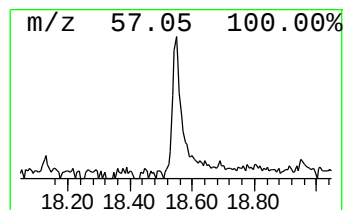
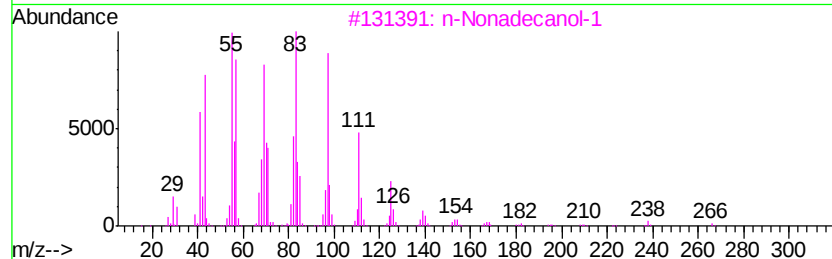
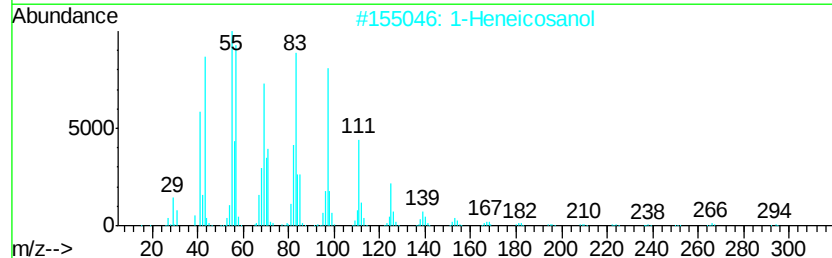
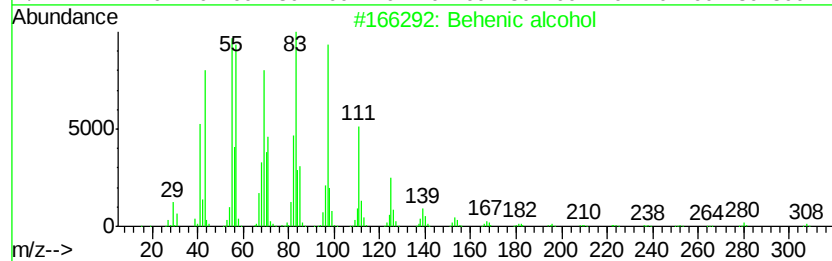
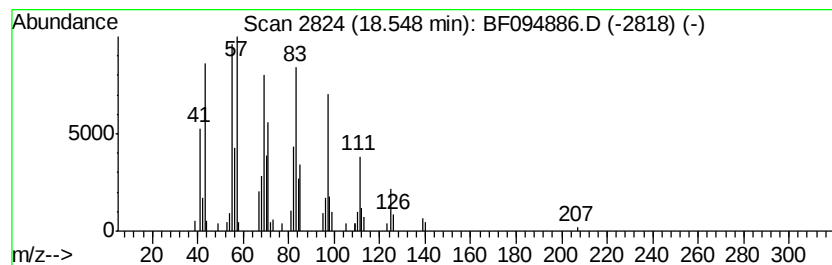
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.55	4.98 ng	191276	Chrysene-d12	18.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93



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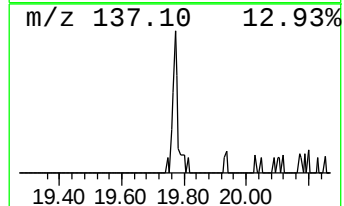
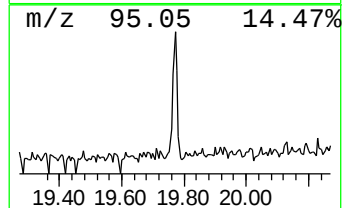
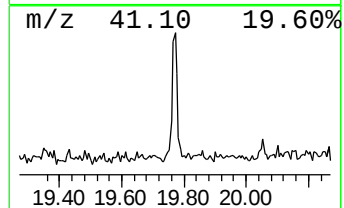
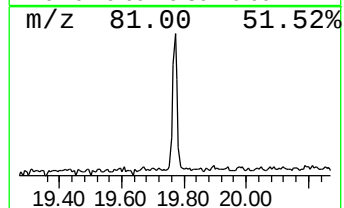
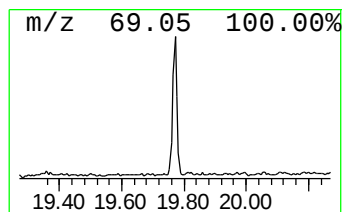
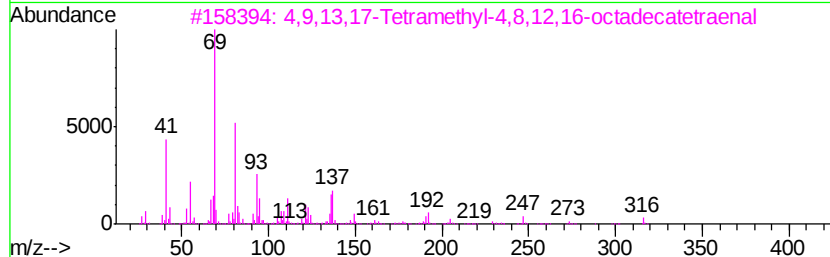
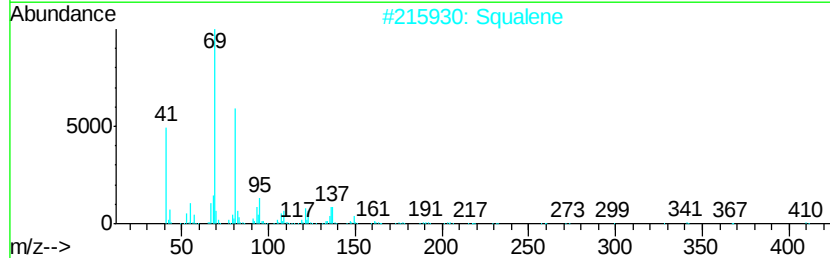
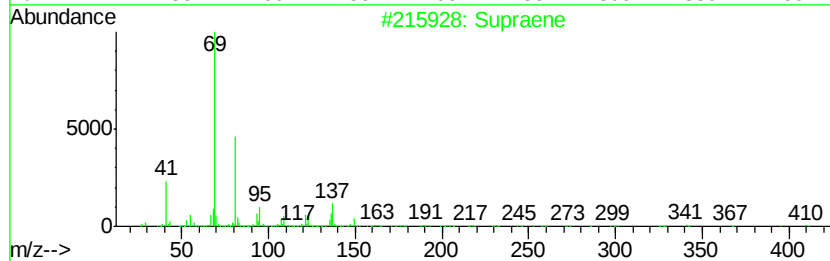
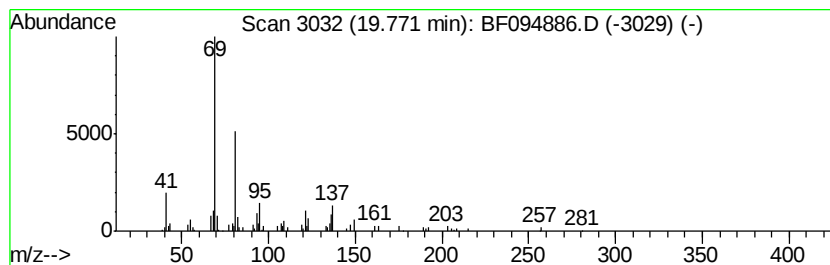
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.75 ng	81872	Perylene-d12	20.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4		Farnesol isomer a	222	C15H26O	1000108-92-4	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	13.4	ng	284293	1	7.72	425172	20.0
unknown7.38	7.38	81.7	ng	1737500	1	7.72	425172	20.0
n-Hexadecanoic acid	15.94	3.8	ng	134243	4	14.97	706415	20.0
Behenic alcohol	18.55	5.0	ng	191276	5	18.63	768190	20.0
Supraene	19.77	2.8	ng	81872	6	20.30	595736	20.0