

Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
 Data File : BF095067.D
 Acq On : 10 May 2017 21:10
 Operator : SJ/MA
 Sample : I3048-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-4923

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	5.007	518	522	538	rBV	126841	267086	10.74%	1.277%
2	5.648	627	631	661	rBV	1142767	2089843	84.06%	9.993%
3	7.254	899	904	919	rBV	1296689	2018749	81.20%	9.653%
4	7.372	919	924	933	rVB	1561201	2293772	92.26%	10.968%
5	7.707	977	981	993	rVB	409617	486863	19.58%	2.328%
6	7.942	1016	1021	1032	rBV	1451759	1692713	68.08%	8.094%
7	8.607	1129	1134	1159	rBV	964747	1314835	52.88%	6.287%
8	9.730	1320	1325	1340	rBV	434129	647657	26.05%	3.097%
9	11.501	1621	1626	1645	rBV	2011471	2486262	100.00%	11.889%
10	12.195	1740	1744	1754	rBV	148460	205702	8.27%	0.984%
11	12.560	1801	1806	1824	rBV2	512804	777151	31.26%	3.716%
12	13.395	1943	1948	1953	rBV	32973	39239	1.58%	0.188%
13	13.854	2021	2026	2039	rBV	940931	1429960	57.51%	6.838%
14	14.171	2076	2080	2083	rBV	36064	43088	1.73%	0.206%
15	14.901	2198	2204	2209	rBV	23502	31892	1.28%	0.152%
16	14.960	2209	2214	2230	rVV2	502889	748106	30.09%	3.577%
17	15.930	2374	2379	2387	rBV	211245	284164	11.43%	1.359%
18	16.001	2387	2391	2397	rVB4	16468	26591	1.07%	0.127%
19	17.012	2560	2563	2568	rBV	98503	132903	5.35%	0.636%
20	17.283	2604	2609	2618	rBV	1906808	2370499	95.34%	11.335%
21	18.536	2817	2822	2831	rBV3	67285	158691	6.38%	0.759%
22	18.630	2834	2838	2846	rBV	521272	693386	27.89%	3.316%
23	19.753	3026	3029	3033	rBV	76859	89848	3.61%	0.430%
24	20.294	3118	3121	3129	rBV	387937	584027	23.49%	2.793%

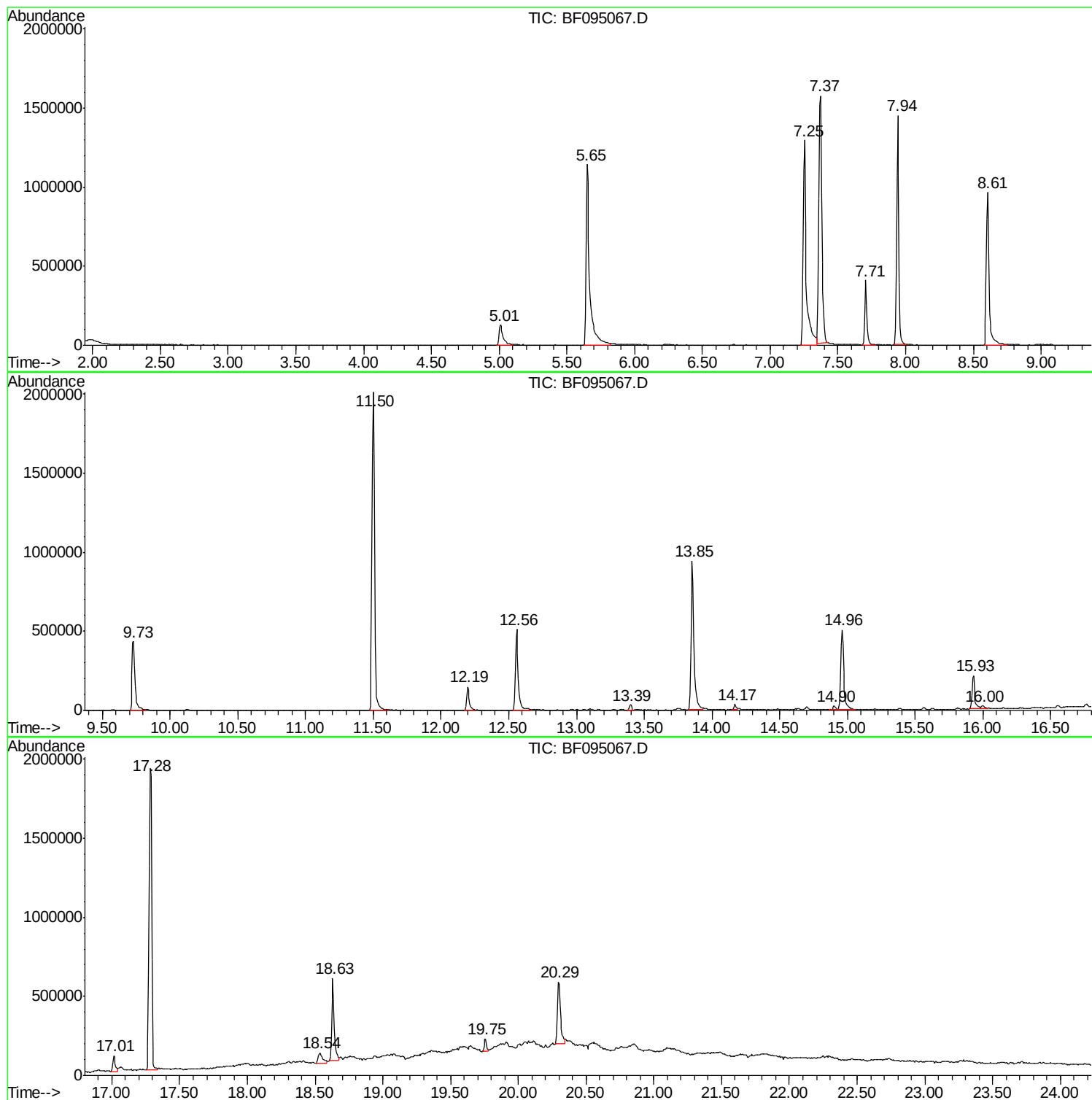
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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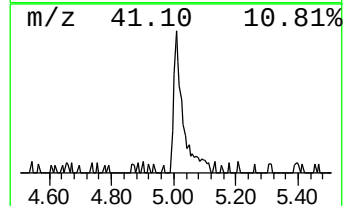
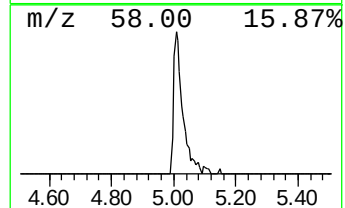
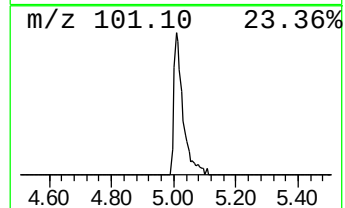
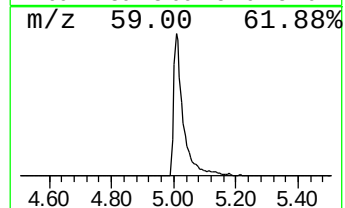
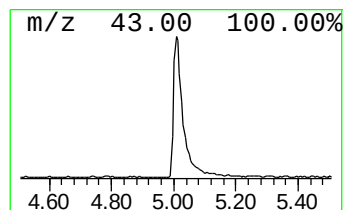
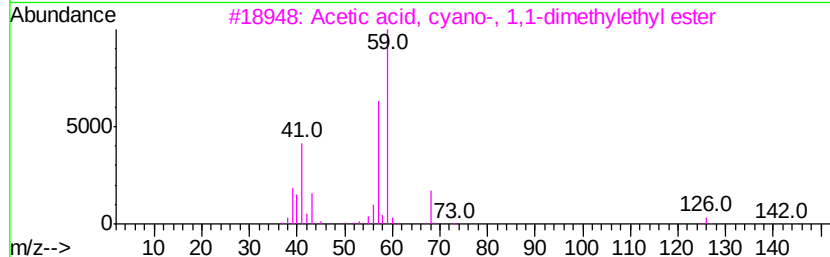
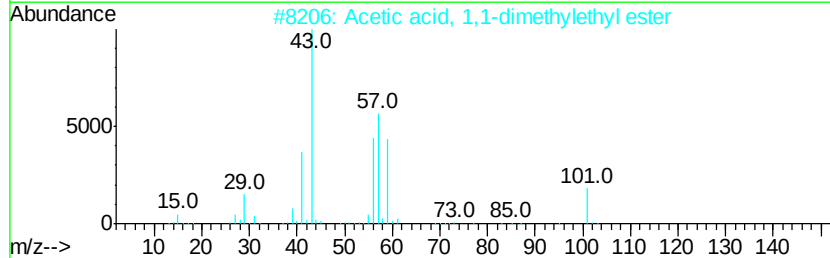
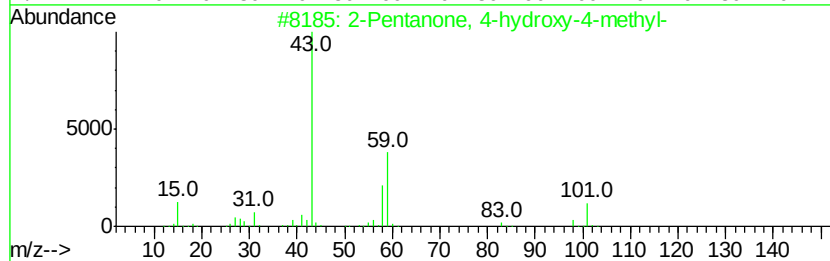
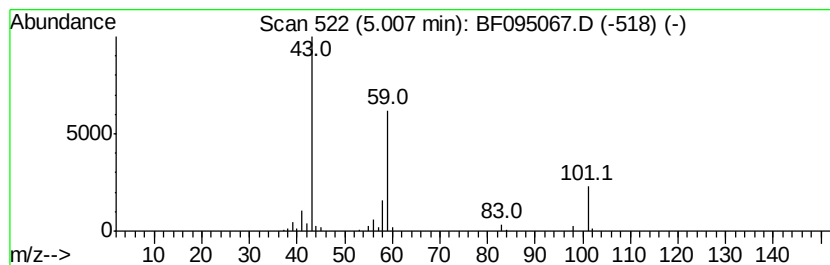
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	10.97 ng	267086	1,4-Dichlorobenzene-d4	7.71

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Butane	58	C4H10	000106-97-8	9



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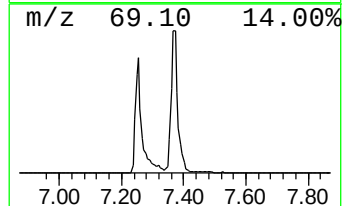
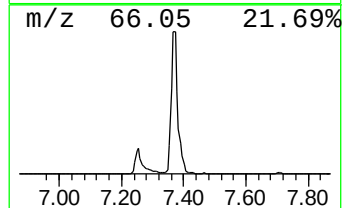
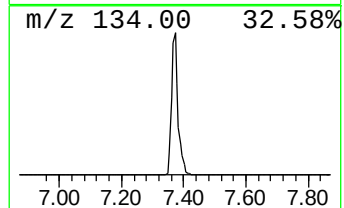
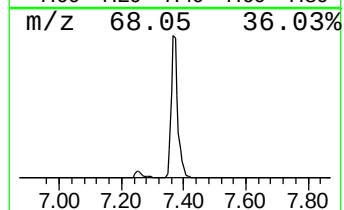
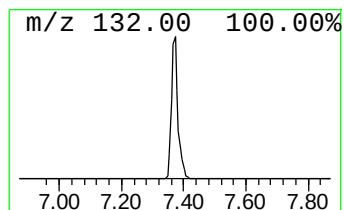
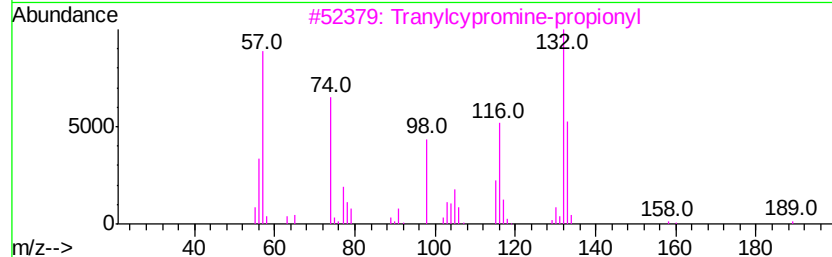
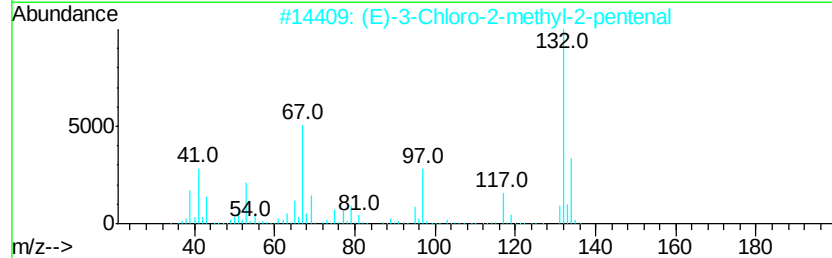
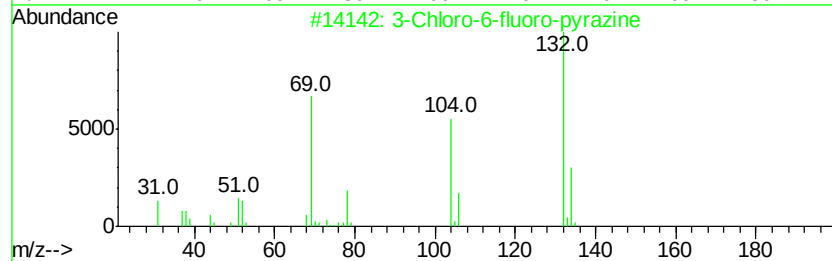
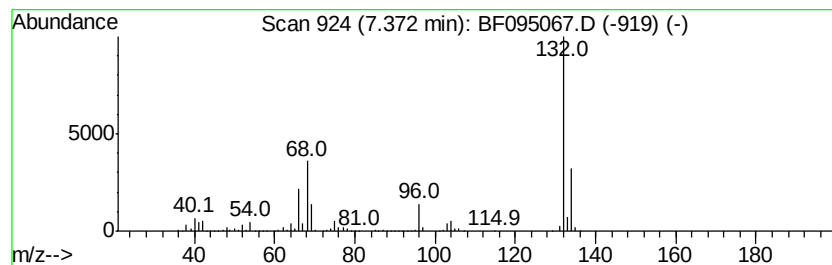
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Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	94.23 ng	2293770	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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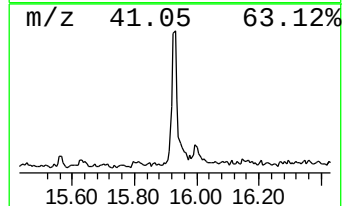
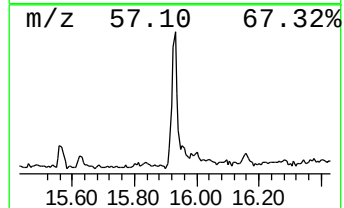
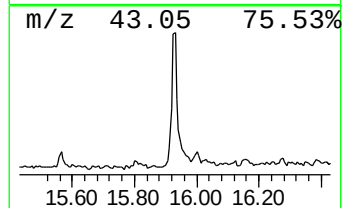
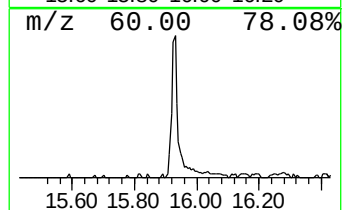
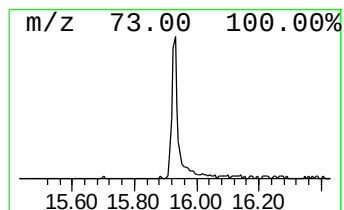
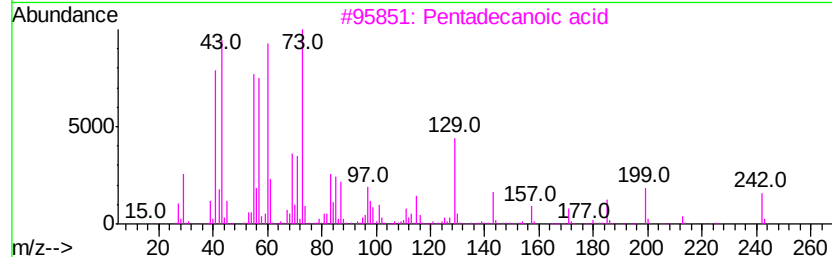
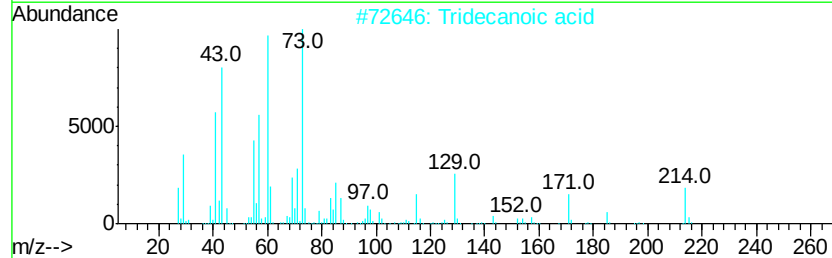
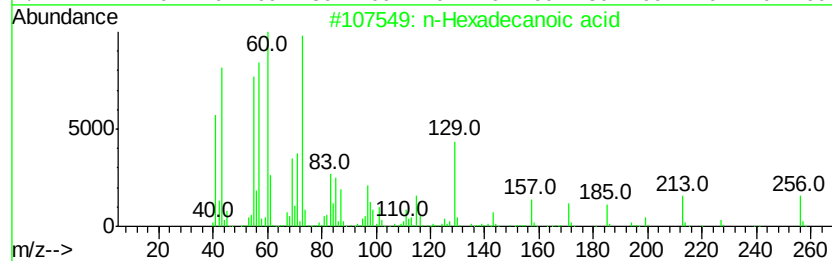
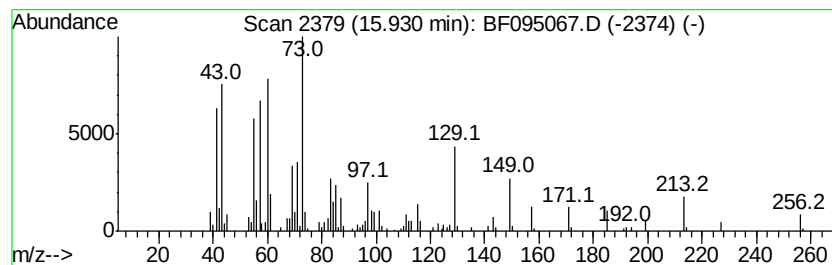
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	7.60 ng	284164	Phenanthrene-d10	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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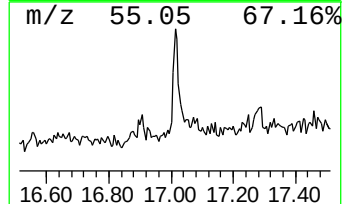
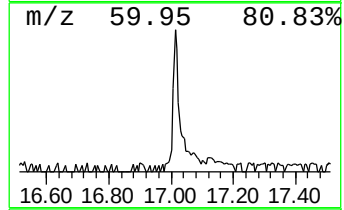
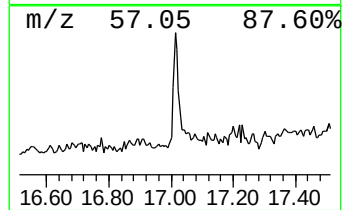
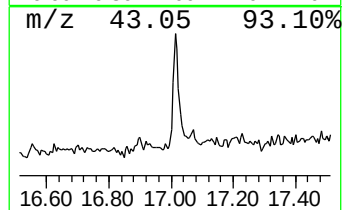
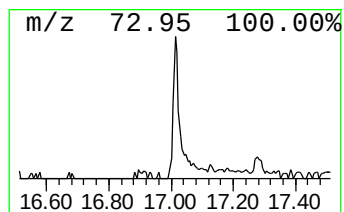
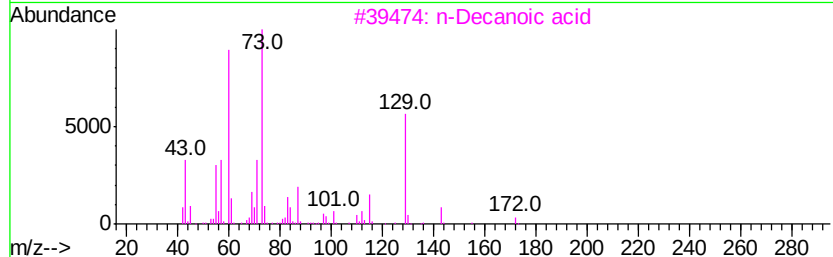
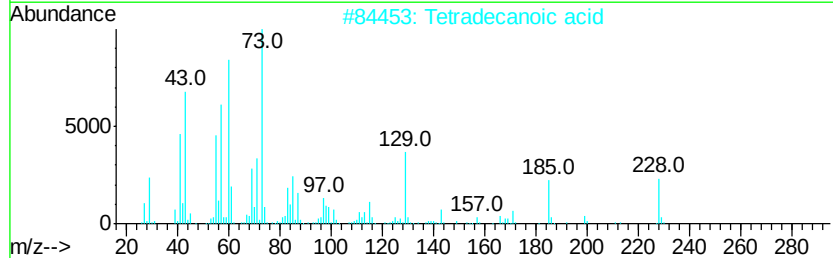
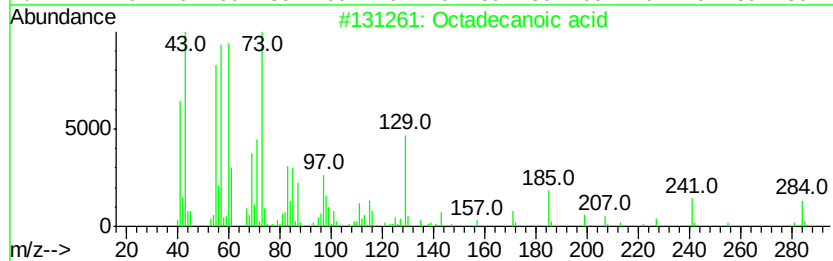
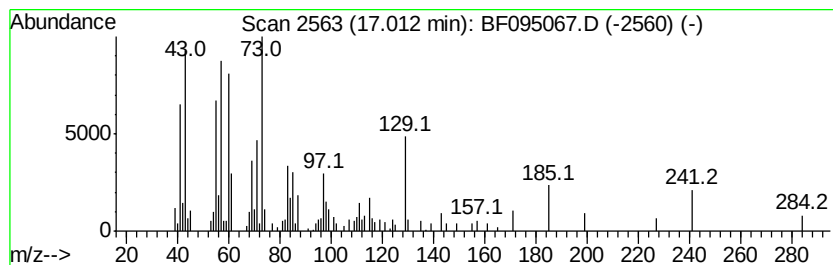
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.01	3.83 ng	132903	Chrysene-d12	18.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3		n-Decanoic acid	172	C10H20O2	000334-48-5	49
4		Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	25
5		5-Acetoxypentadecane	270	C17H34O2	1000245-62-3	14



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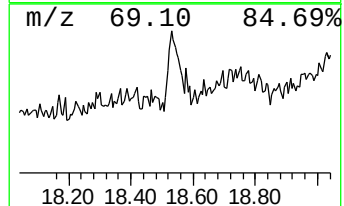
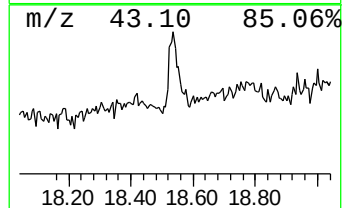
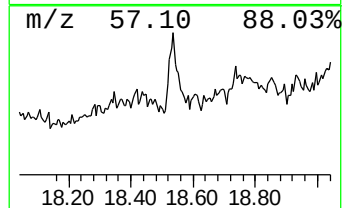
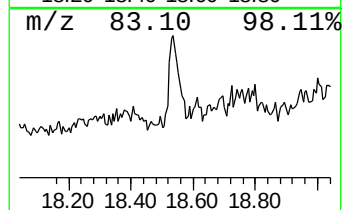
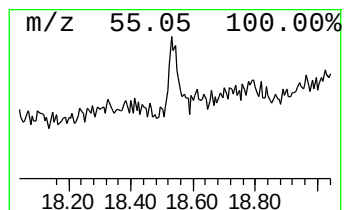
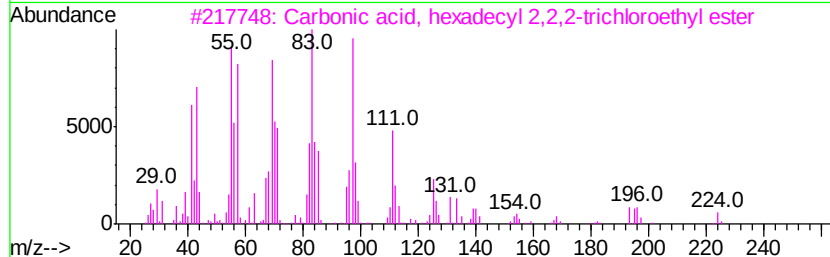
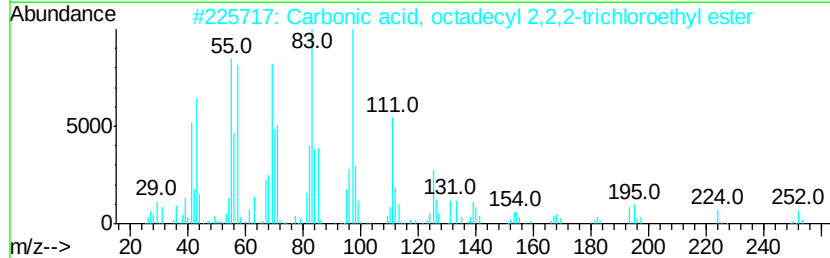
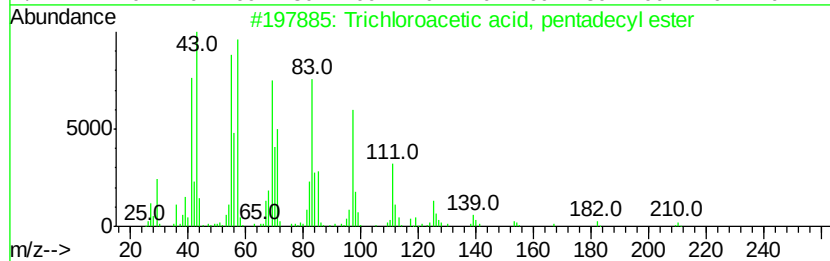
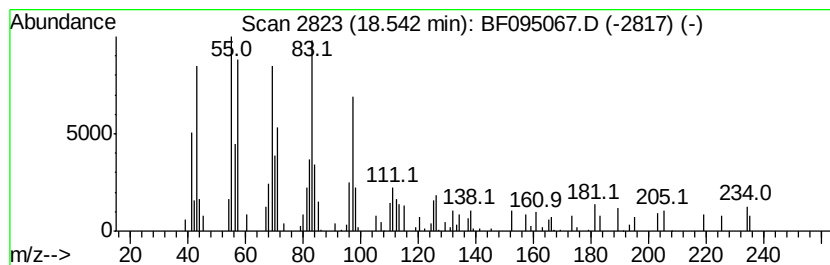
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Peak Number 6 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.54	4.58 ng	158691	Chrysene-d12	18.63	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
2	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87
3	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	87
4	Octacosanol	410	C28H58O	000557-61-9	86
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81



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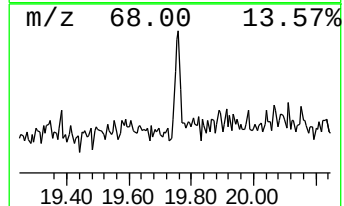
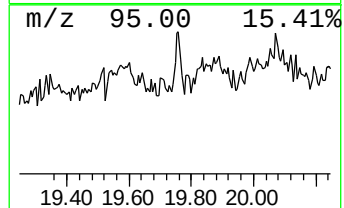
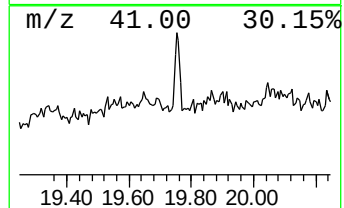
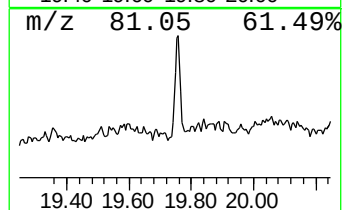
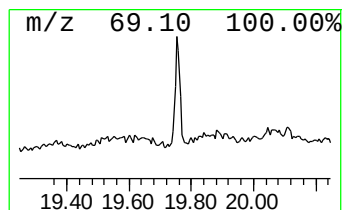
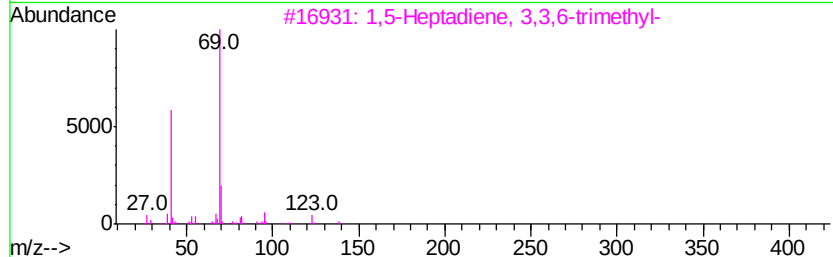
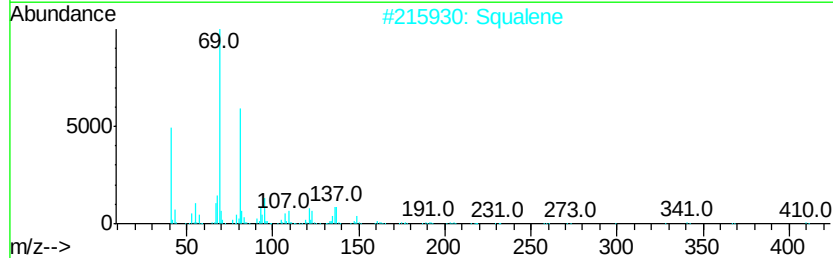
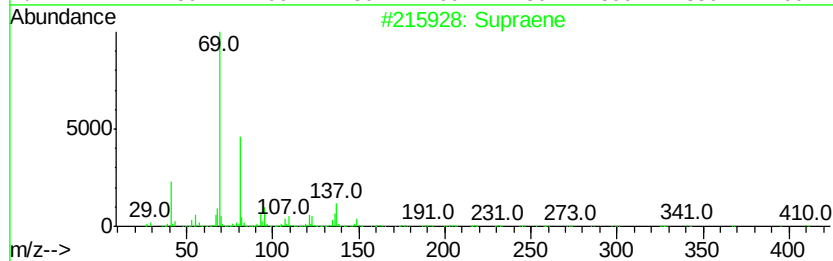
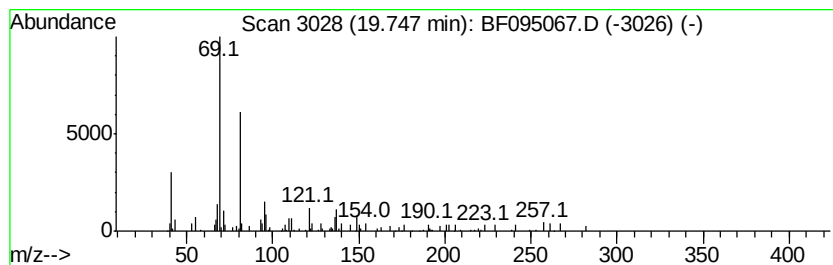
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RO-4923

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

Peak Number 7 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.75	3.08 ng	89848	Perylene-d12	20.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Supraene		410 C30H50	007683-64-9 86
2	Squalene		410 C30H50	000111-02-4 80
3	1,5-Heptadiene, 3,3,6-trimethyl-		138 C10H18	035387-63-4 53
4	2,6-Octadien-1-ol, 3,7-dimethyl-...		154 C10H18O	000106-25-2 53
5	1,6-Octadiene, 3,5-dimethyl-, tr...		138 C10H18	074630-87-8 53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051017\
Data File : BF095067.D
Acq On : 10 May 2017 21:10
Operator : SJ/MA
Sample : I3048-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-4923

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	11.0	ng	267086	1	7.71	486863	20.0
unknown7.37	7.37	94.2	ng	2293770	1	7.71	486863	20.0
n-Hexadecanoic acid	15.93	7.6	ng	284164	4	14.96	748106	20.0
Octadecanoic acid	17.01	3.8	ng	132903	5	18.63	693386	20.0
Trichloroacetic a...	18.54	4.6	ng	158691	5	18.63	693386	20.0
Supraene	19.75	3.1	ng	89848	6	20.29	584027	20.0