

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052517\
 Data File : BF095432.D
 Acq On : 25 May 2017 19:51
 Operator : SJ/MA
 Sample : I3347-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-11931/VNJ-208/153/341/132

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	5.107	536	539	554	rBV2	88459	211126	7.51%	0.908%
2	5.707	637	641	680	rBV	1076178	2499911	88.97%	10.749%
3	7.290	906	910	926	rBV	1238828	2253434	80.20%	9.689%
4	7.413	926	931	953	rVB	1648187	2809691	100.00%	12.081%
5	7.742	983	987	997	rBV	483212	589893	20.99%	2.536%
6	7.984	1023	1028	1048	rVB	1522790	1931583	68.75%	8.305%
7	8.648	1136	1141	1168	rBV	815623	1494837	53.20%	6.428%
8	9.772	1327	1332	1350	rBV	406655	792234	28.20%	3.406%
9	11.536	1627	1632	1652	rBV	1804395	2767186	98.49%	11.898%
10	12.236	1746	1751	1761	rBV	362937	574019	20.43%	2.468%
11	12.601	1808	1813	1825	rBV2	574145	867629	30.88%	3.731%
12	13.430	1950	1954	1958	rBV	47752	50739	1.81%	0.218%
13	13.789	2005	2015	2019	rBV4	16615	39130	1.39%	0.168%
14	13.901	2029	2034	2050	rBV	773127	1385972	49.33%	5.959%
15	14.201	2082	2085	2088	rBV	49685	61203	2.18%	0.263%
16	14.936	2206	2210	2213	rBV	32154	41049	1.46%	0.177%
17	15.007	2215	2222	2226	rBV	429333	641461	22.83%	2.758%
18	15.842	2360	2364	2373	rVV5	23620	50697	1.80%	0.218%
19	15.960	2378	2384	2396	rVB5	95721	187269	6.67%	0.805%
20	16.789	2521	2525	2535	rBV	157813	218847	7.79%	0.941%
21	17.048	2565	2569	2573	rBV5	26561	37072	1.32%	0.159%
22	17.089	2573	2576	2584	rVB	173332	223701	7.96%	0.962%
23	17.318	2611	2615	2625	rBV	1360285	1683679	59.92%	7.240%
24	17.559	2652	2656	2662	rVB2	18894	30931	1.10%	0.133%
25	17.695	2674	2679	2683	rVB5	28120	41460	1.48%	0.178%
26	18.559	2822	2826	2836	rVB3	52048	101916	3.63%	0.438%
27	18.677	2840	2846	2851	rBV2	458195	681540	24.26%	2.931%
28	18.965	2892	2895	2900	rBV5	25010	34796	1.24%	0.150%
29	19.789	3032	3035	3041	rBV	83573	100434	3.57%	0.432%
30	19.953	3059	3063	3066	rBV	63001	95910	3.41%	0.412%
31	20.247	3110	3113	3116	rBV	50429	66388	2.36%	0.285%
32	20.306	3120	3123	3127	rVV	74180	97451	3.47%	0.419%
33	20.353	3127	3131	3141	rVV	334127	482555	17.17%	2.075%
34	21.559	3333	3336	3340	rBV5	31274	47919	1.71%	0.206%

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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 >
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35	21.724	3359	3364	3367	rVB5	31488	63014	2.24%	0.271%
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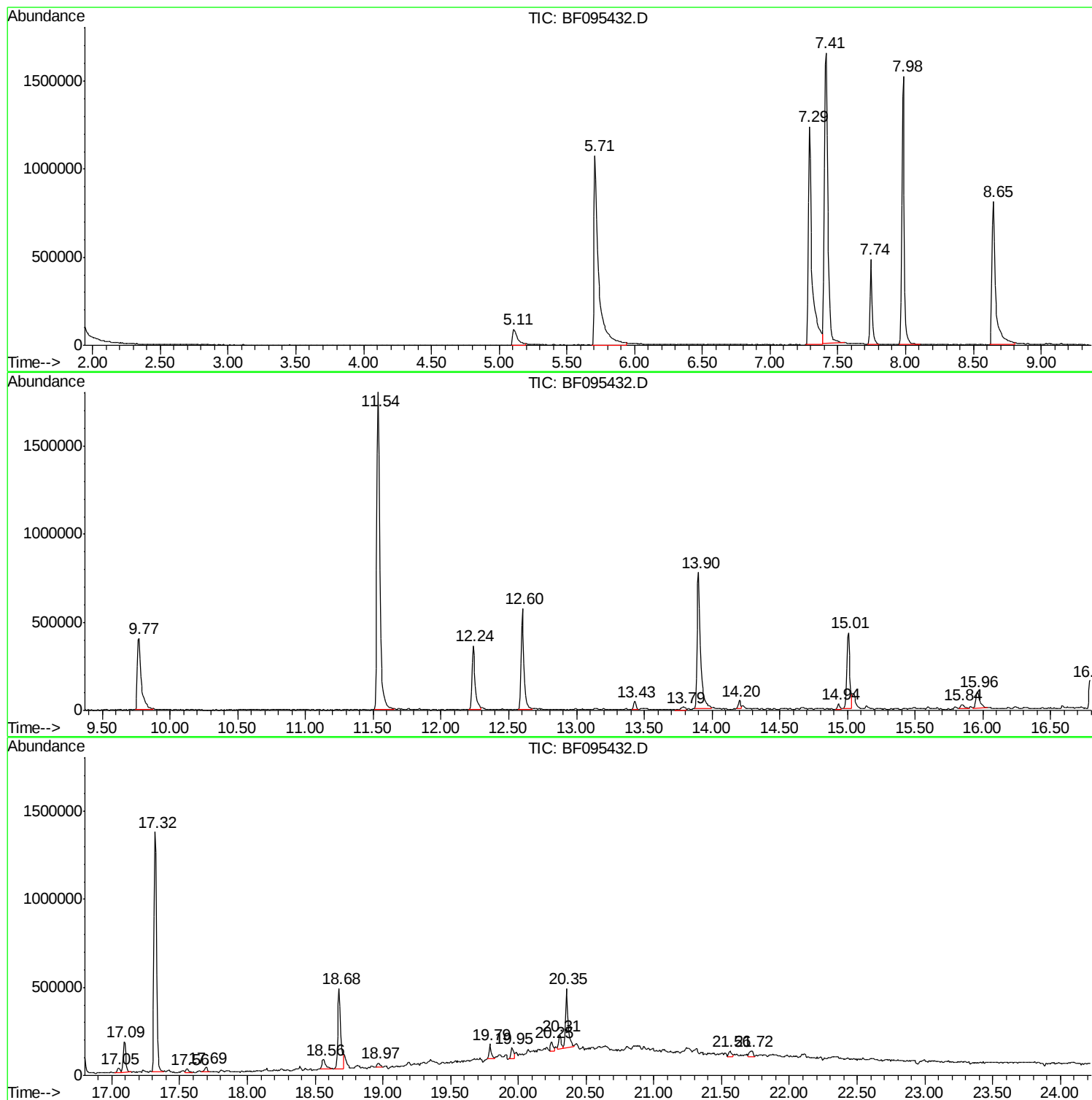
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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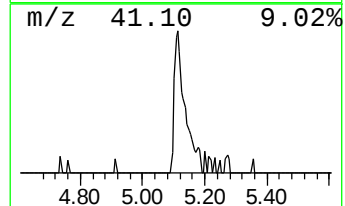
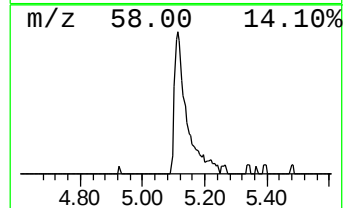
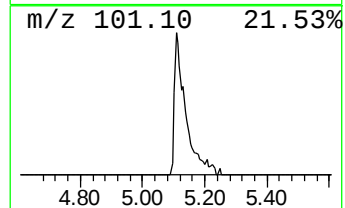
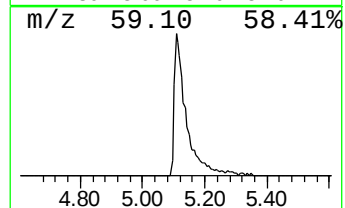
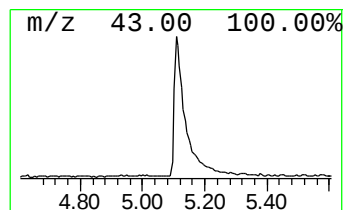
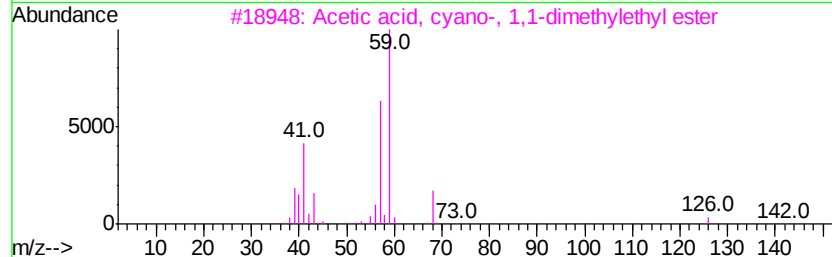
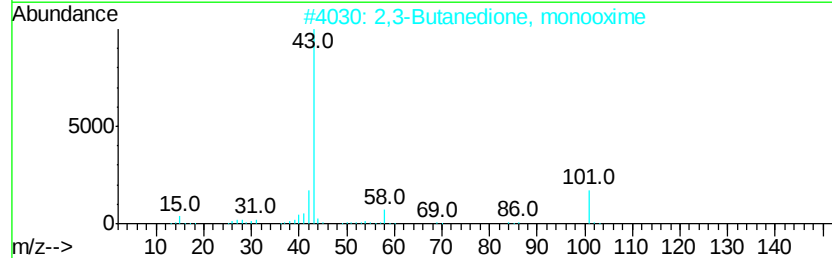
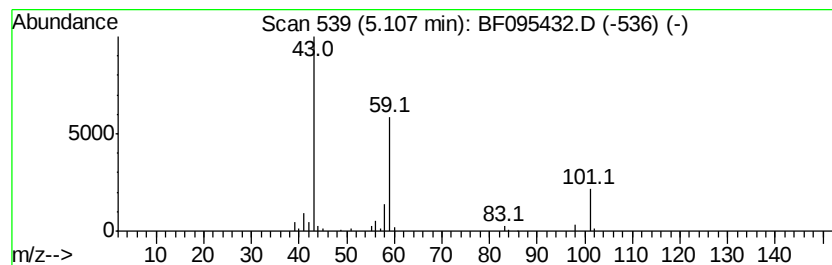
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	7.16 ng	211126	1,4-Dichlorobenzene-d4	7.74

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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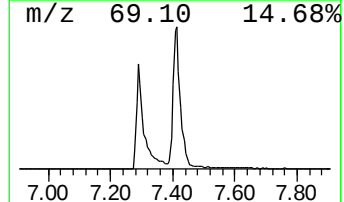
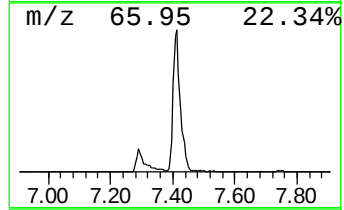
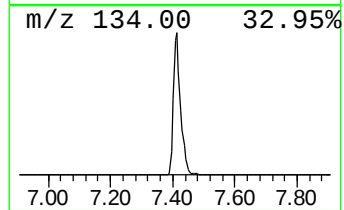
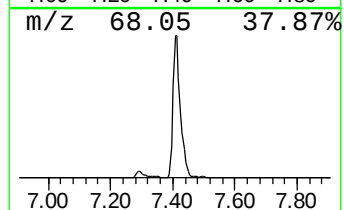
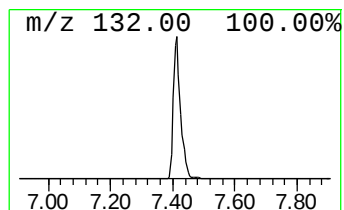
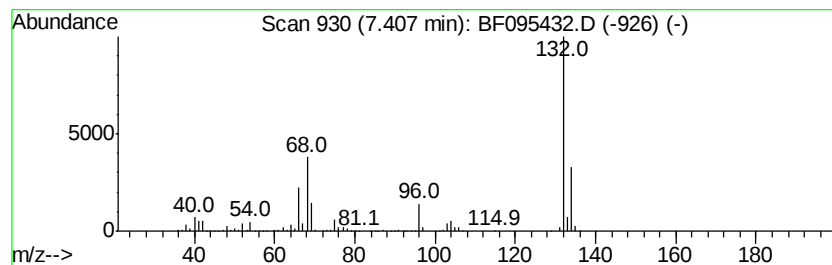
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	95.26 ng	2809690	1,4-Dichlorobenzene-d4	7.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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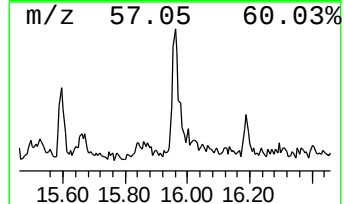
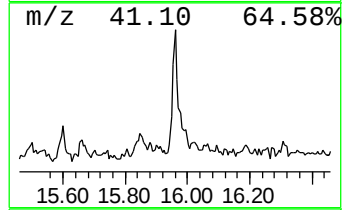
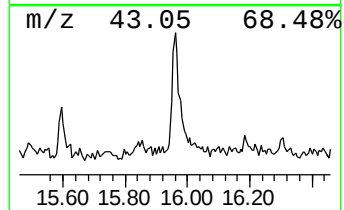
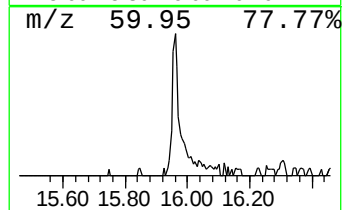
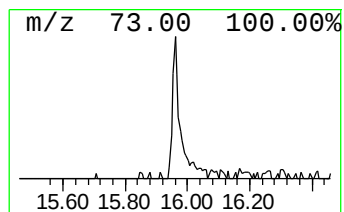
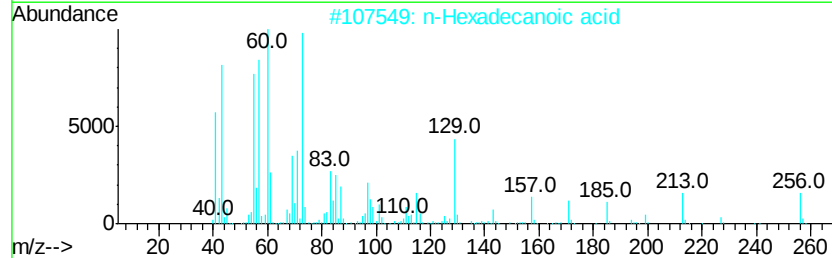
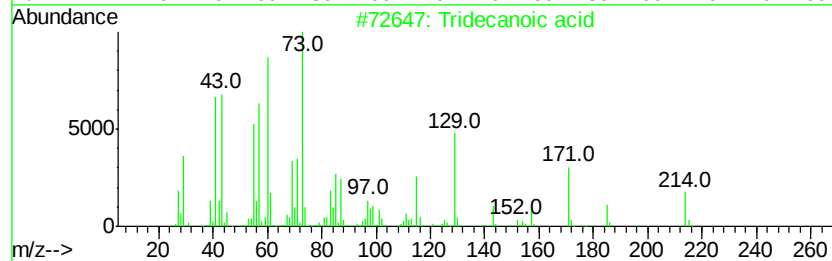
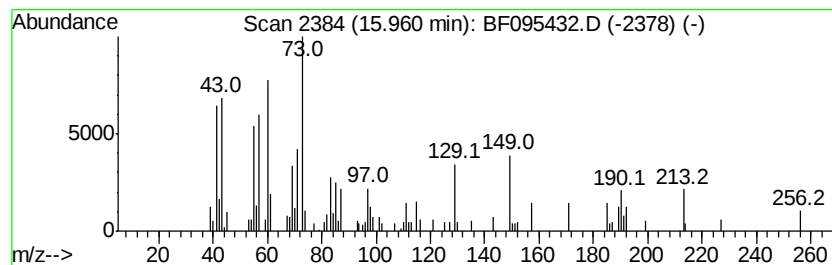
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.96	5.84 ng	187269	Phenanthrene-d10		15.01
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	91
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	43



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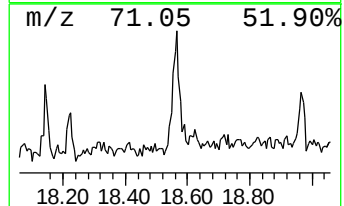
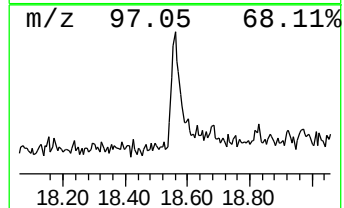
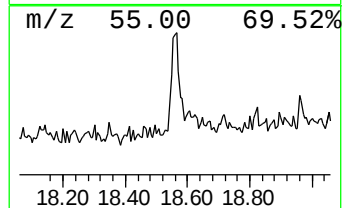
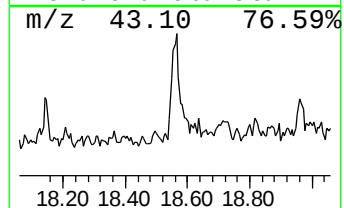
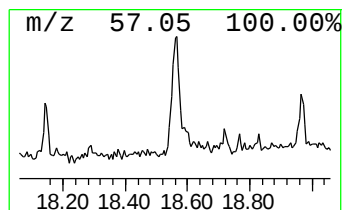
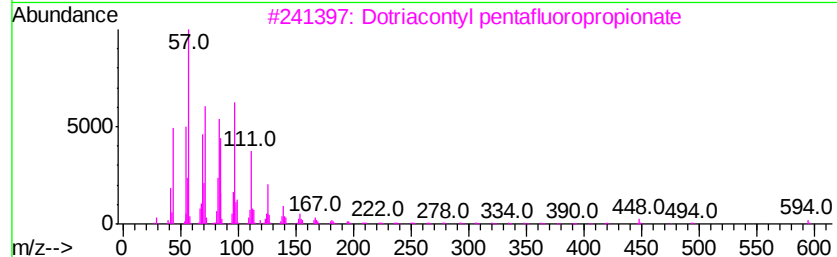
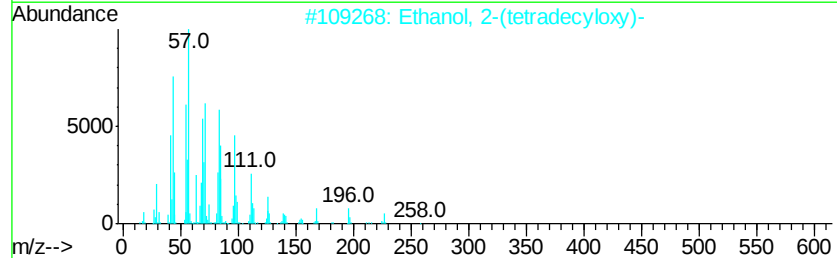
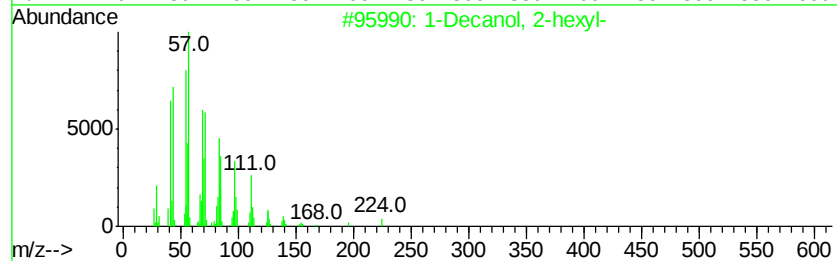
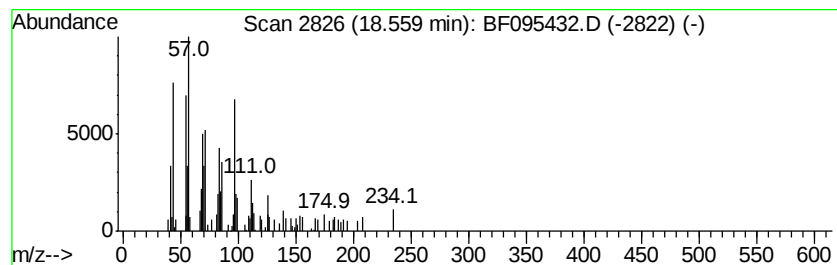
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Peak Number 5 1-Decanol, 2-hexyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.99 ng	101916	Chrysene-d12	18.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6	74
2	Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1	68
3	Dotriacontyl pentafluoropropionate	612 C35H65F5O2	1000351-81-4	64
4	Tetrapentacontane, 1,54-dibromo-	915 C54H108Br2	1000156-09-4	58
5	1-Dodecanol, 2-hexyl-	270 C18H38O	110225-00-8	58



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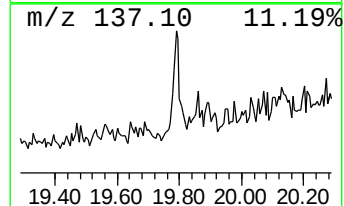
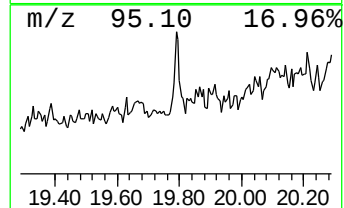
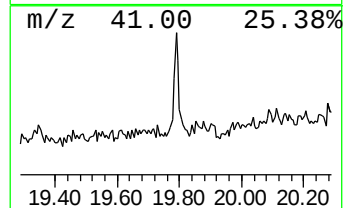
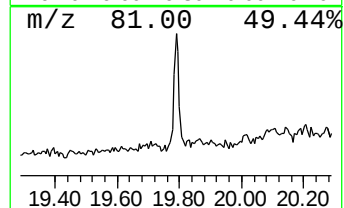
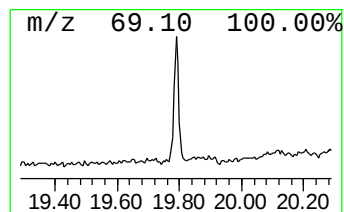
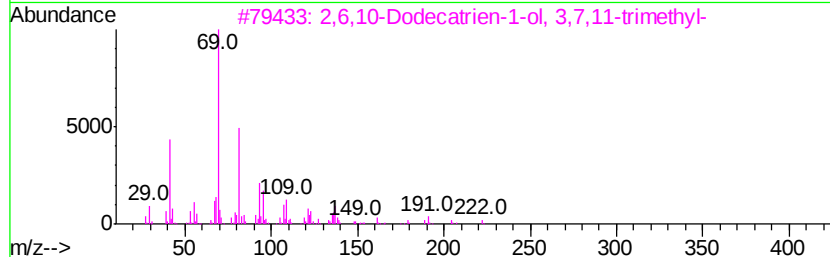
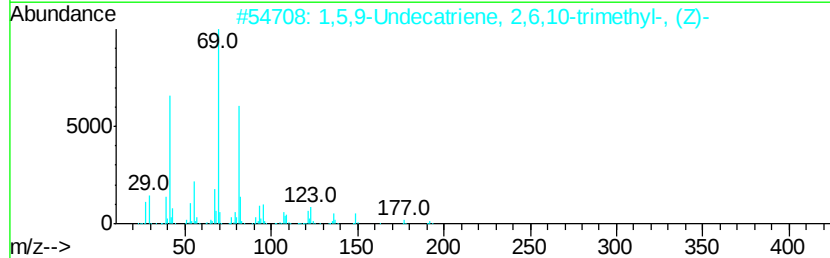
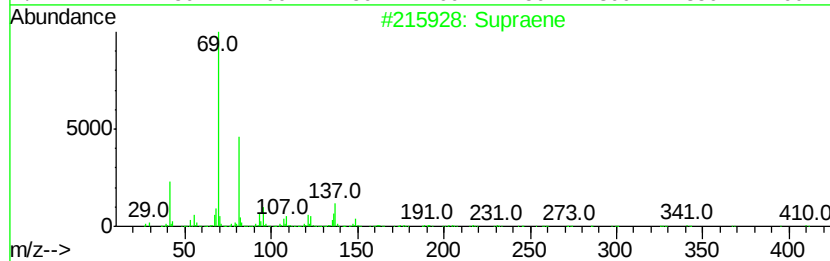
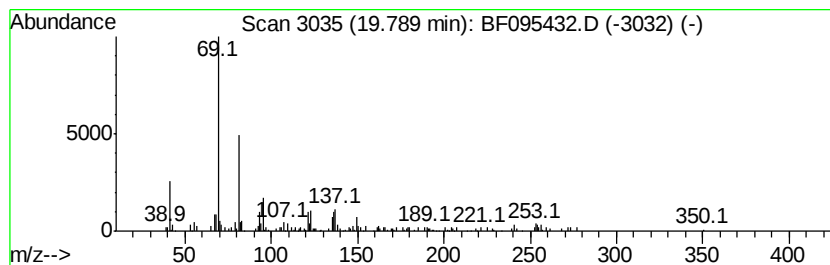
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	4.16 ng	100434	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	86
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
4		Squalene	410	C30H50	000111-02-4	64
5		1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	59



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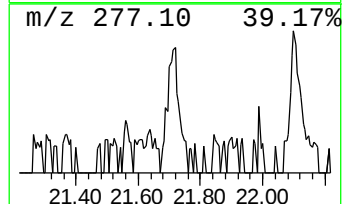
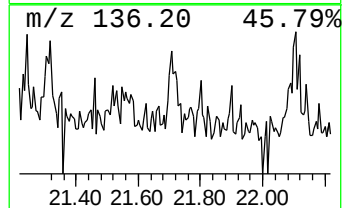
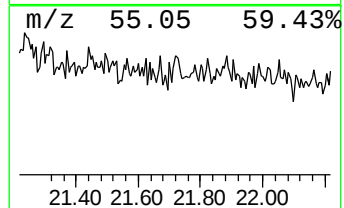
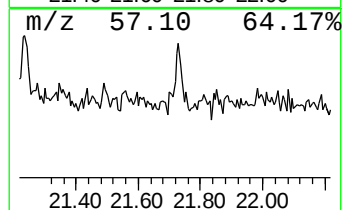
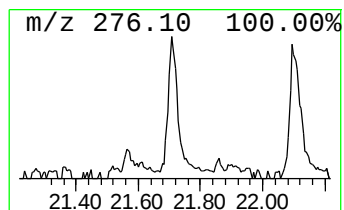
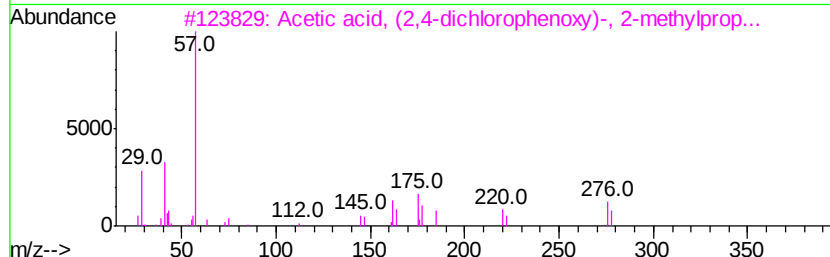
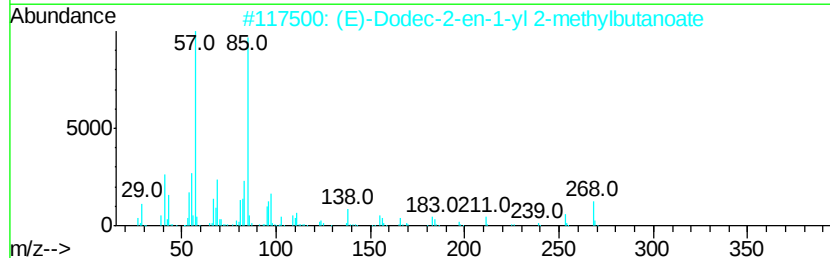
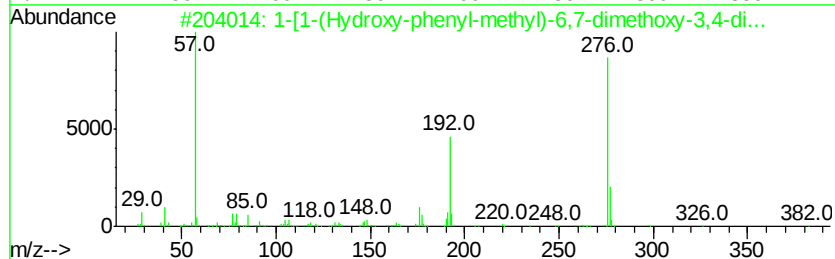
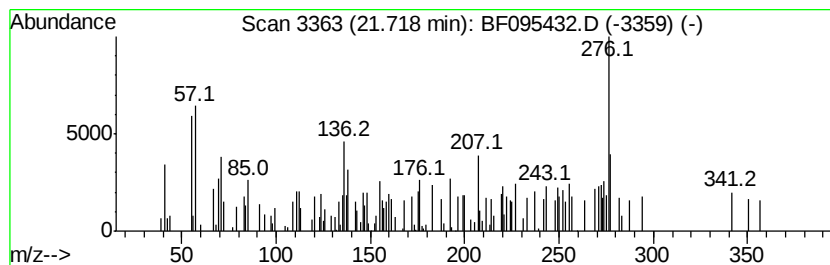
Instrument :
BNA_F
ClientSampleId :
72-11931/VNJ-208/153/341/132

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 8 unknown21.72 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.72	2.61 ng	63014	Perylene-d12	20.35		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-[1-(Hydroxy-phenyl-methyl)-6,7...	383	C23H29N04	114609-12-0	27
2		(E)-Dodec-2-en-1-yl 2-methylbuta...	268	C17H32O2	1000372-81-2	10
3		Acetic acid, (2,4-dichlorophenox...	276	C12H14Cl2O3	001713-15-1	10
4		Pipobroman	354	C10H16Br2N2O2	000054-91-1	10
5		Fumaric acid, dodecyl tetrahydro...	368	C21H36O5	1000330-58-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052517\
Data File : BF095432.D
Acq On : 25 May 2017 19:51
Operator : SJ/MA
Sample : I3347-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
72-11931/VNJ-208/153/341/132

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	7.2	ng	211126	1	7.74	589893	20.0
unknown7.41	7.41	95.3	ng	2809690	1	7.74	589893	20.0
Tridecanoic acid	15.96	5.8	ng	187269	4	15.01	641461	20.0
1-Decanol, 2-hexyl-	18.56	3.0	ng	101916	5	18.68	681540	20.0
Supraene	19.79	4.2	ng	100434	6	20.35	482555	20.0
unknown21.72	21.72	2.6	ng	63014	6	20.35	482555	20.0