

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052517\
 Data File : BF095431.D
 Acq On : 25 May 2017 19:19
 Operator : SJ/MA
 Sample : I3332-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-25COMP

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	552	rBV	74795	176241	7.25%	0.852%
2	5.713	638	642	674	rBV	839322	2138915	88.03%	10.334%
3	7.290	906	910	926	rBV	981845	1977856	81.40%	9.556%
4	7.413	926	931	951	rVB	1408956	2429651	100.00%	11.739%
5	7.742	983	987	1000	rVB	453754	566392	23.31%	2.737%
6	7.984	1023	1028	1041	rBV	1287852	1726220	71.05%	8.340%
7	8.648	1136	1141	1170	rBV	685941	1318649	54.27%	6.371%
8	9.766	1327	1331	1356	rBV	412211	783974	32.27%	3.788%
9	11.536	1627	1632	1650	rBV	1546624	2314716	95.27%	11.184%
10	11.683	1653	1657	1664	rVB8	15046	27388	1.13%	0.132%
11	12.236	1746	1751	1763	rBV	415685	656647	27.03%	3.173%
12	12.454	1784	1788	1793	rVB5	20625	26932	1.11%	0.130%
13	12.601	1807	1813	1820	rBV2	560338	865432	35.62%	4.181%
14	13.142	1899	1905	1911	rVV8	18107	34198	1.41%	0.165%
15	13.430	1950	1954	1958	rVB	49003	57687	2.37%	0.279%
16	13.789	2009	2015	2020	rVB5	17142	32724	1.35%	0.158%
17	13.901	2029	2034	2053	rBV	743316	1342247	55.24%	6.485%
18	14.201	2080	2085	2095	rVV2	66981	127649	5.25%	0.617%
19	14.930	2206	2209	2213	rBV	34883	37568	1.55%	0.182%
20	15.001	2215	2221	2237	rVV2	476337	774107	31.86%	3.740%
21	15.489	2301	2304	2308	rBV5	22390	34967	1.44%	0.169%
22	15.595	2318	2322	2325	rBV3	26409	39793	1.64%	0.192%
23	15.960	2378	2384	2393	rBV5	99322	181431	7.47%	0.877%
24	16.583	2487	2490	2494	rBV5	19405	31668	1.30%	0.153%
25	16.795	2522	2526	2531	rBV	56638	86236	3.55%	0.417%
26	17.095	2573	2577	2581	rVB	62062	79780	3.28%	0.385%
27	17.318	2611	2615	2625	rBV	1306565	1528316	62.90%	7.384%
28	18.559	2822	2826	2831	rBV2	54323	80695	3.32%	0.390%
29	18.677	2842	2846	2858	rBV	391715	571225	23.51%	2.760%
30	19.118	2917	2921	2923	rBV5	19147	34933	1.44%	0.169%
31	19.353	2957	2961	2964	rBV5	33143	51844	2.13%	0.250%
32	19.789	3032	3035	3040	rBV	83097	84850	3.49%	0.410%
33	20.353	3128	3131	3140	rBV	330740	476298	19.60%	2.301%

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ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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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 >
Peak separation: 5

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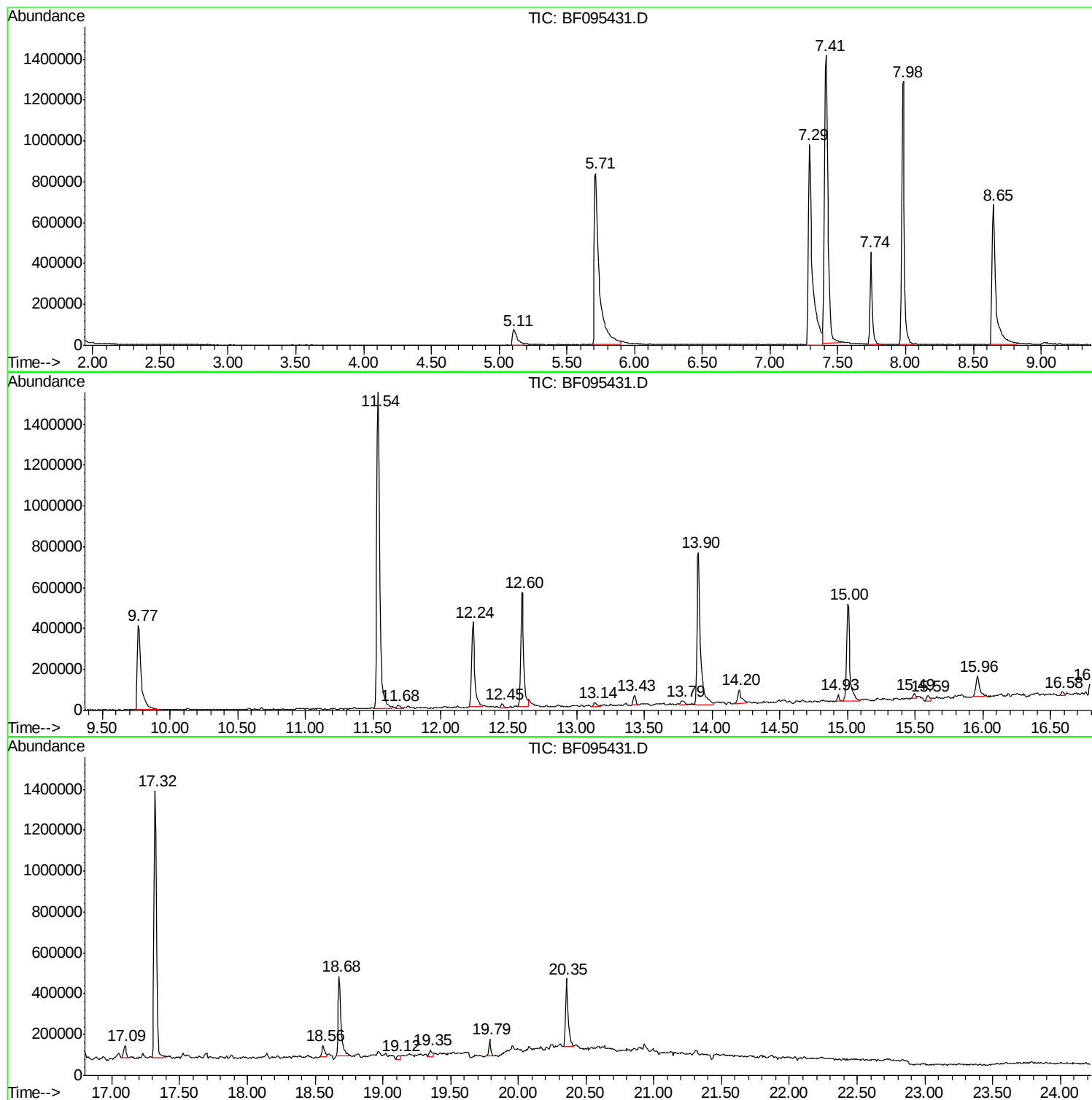
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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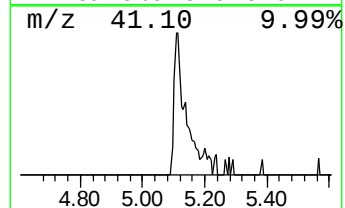
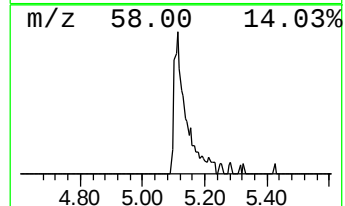
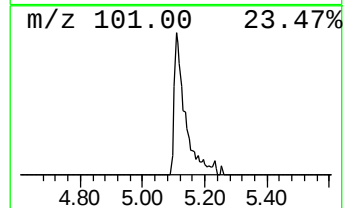
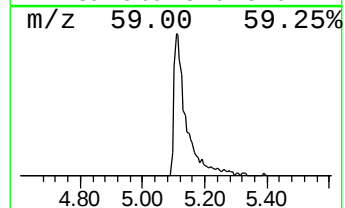
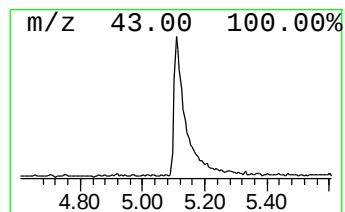
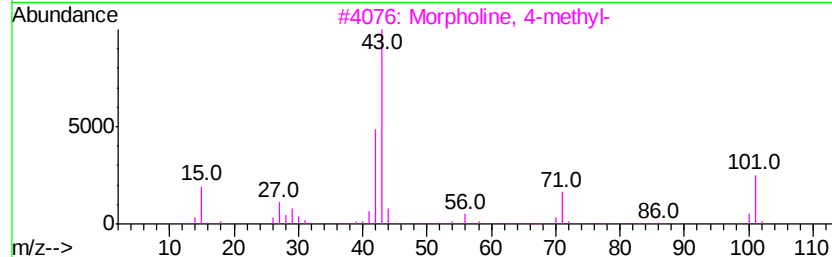
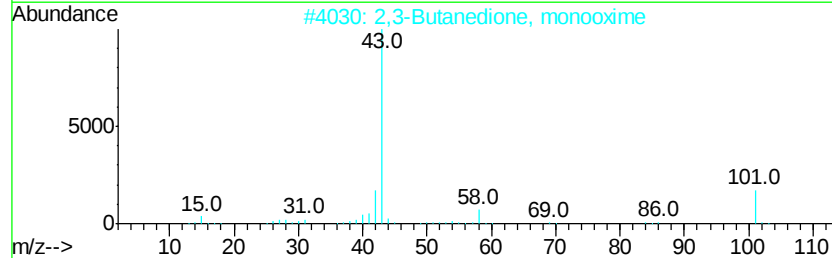
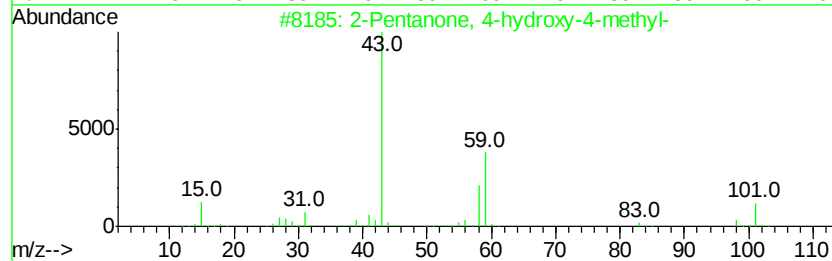
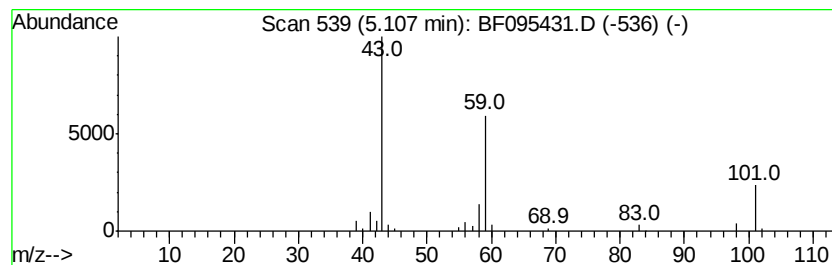
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	6.22 ng	176241	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	64
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Butane	58	C4H10	000106-97-8	9



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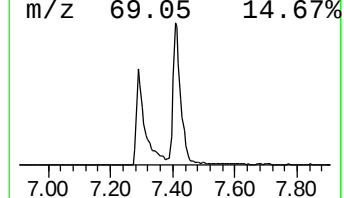
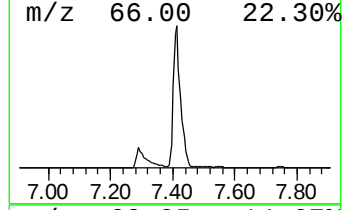
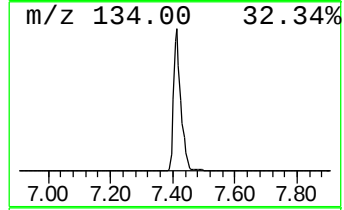
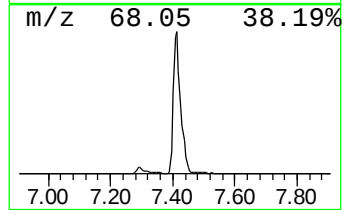
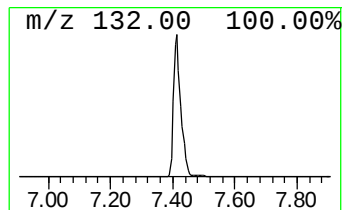
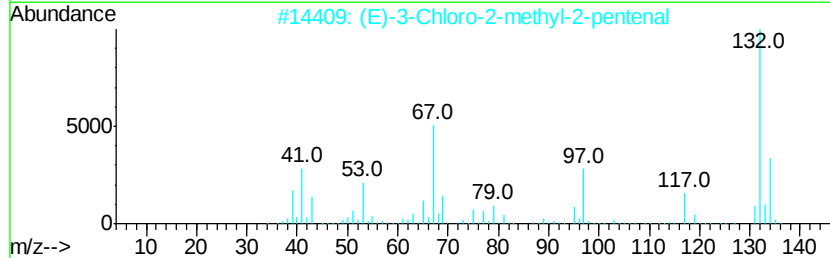
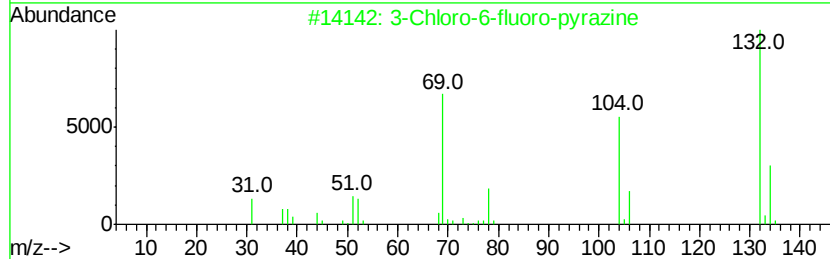
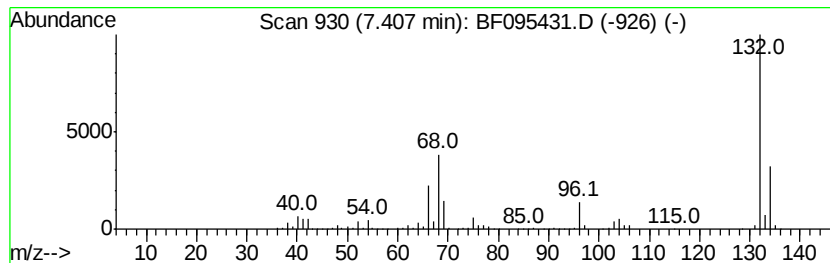
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.41 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	85.79 ng	2429650	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	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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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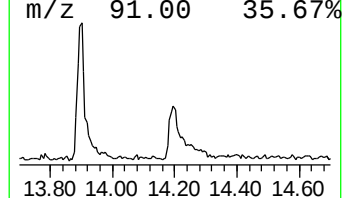
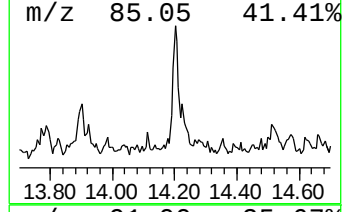
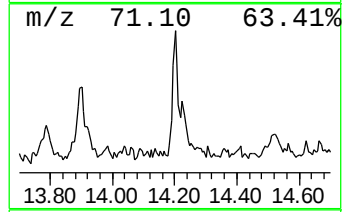
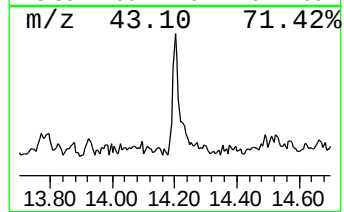
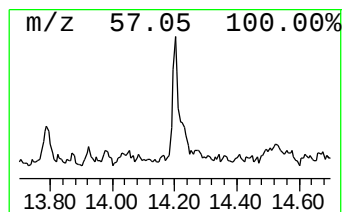
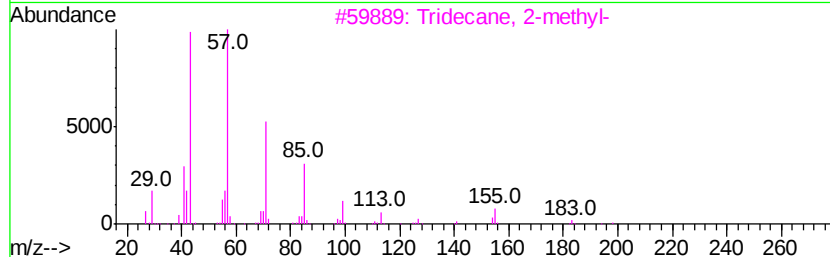
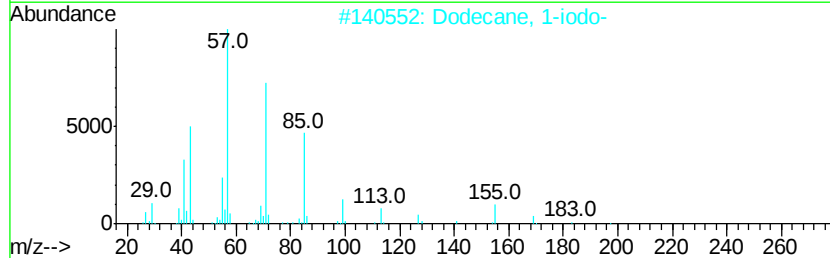
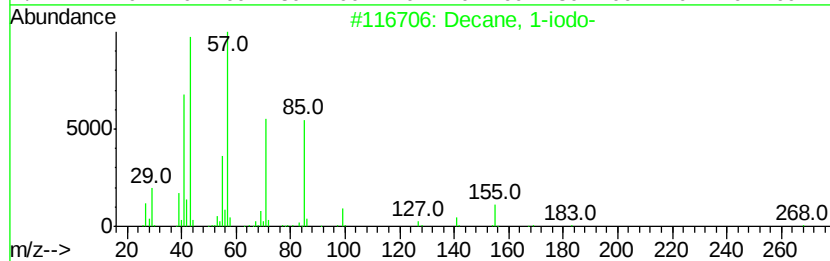
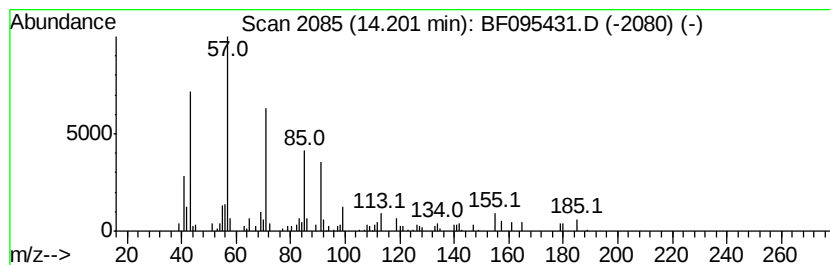
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Decane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.20	3.30 ng	127649	Phenanthrene-d10	15.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1-iodo-	268	C10H21I	002050-77-3	72
2			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	72
3			Tridecane, 2-methyl-	198	C14H30	001560-96-9	64
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5			Octadecane	254	C18H38	000593-45-3	59



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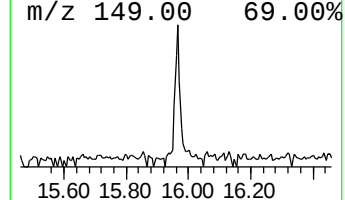
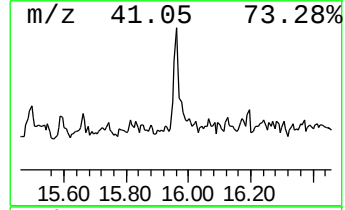
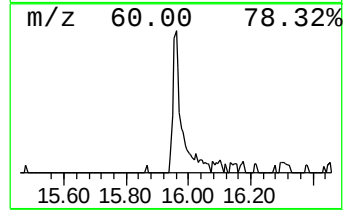
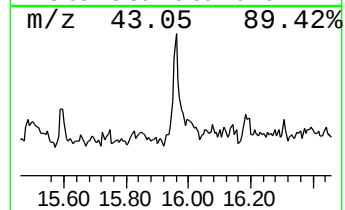
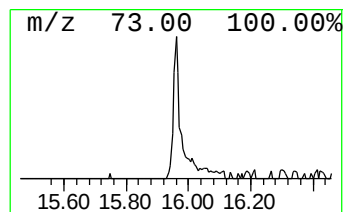
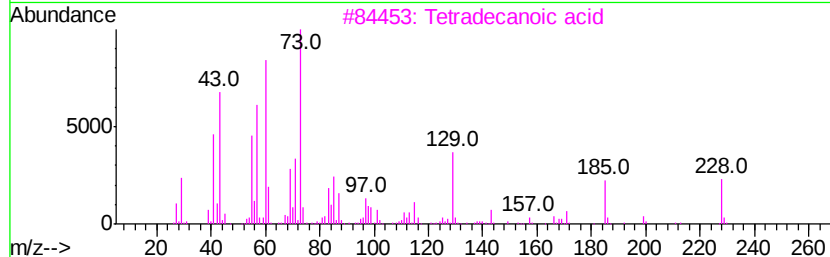
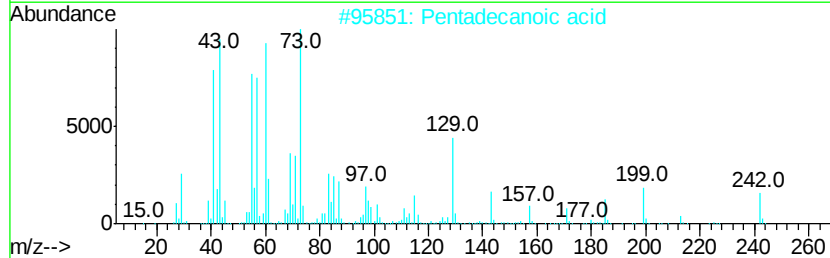
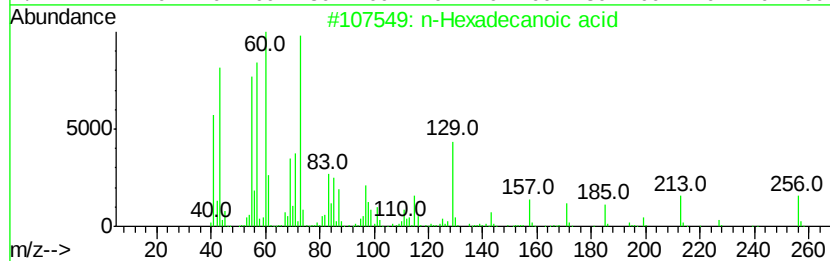
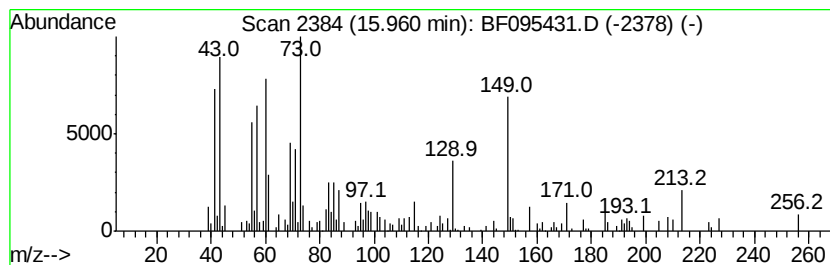
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	4.69 ng	181431	Phenanthrene-d10	15.00

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Undecanoic acid	186	C11H22O2	000112-37-8	49
5		Trehalose	342	C12H22O11	000099-20-7	27



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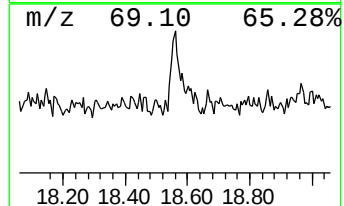
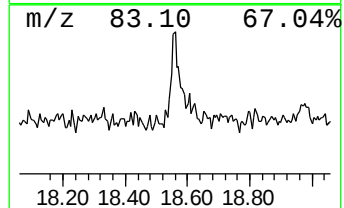
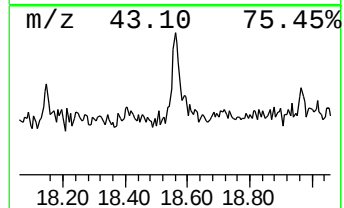
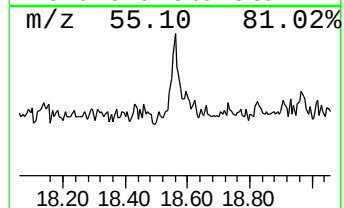
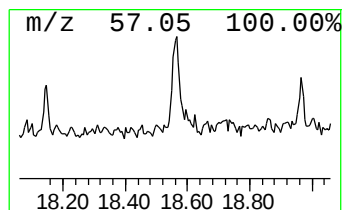
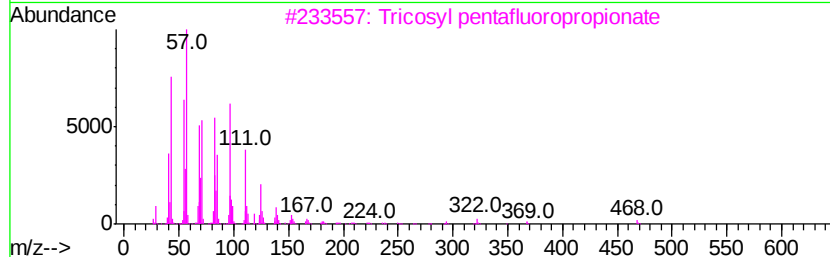
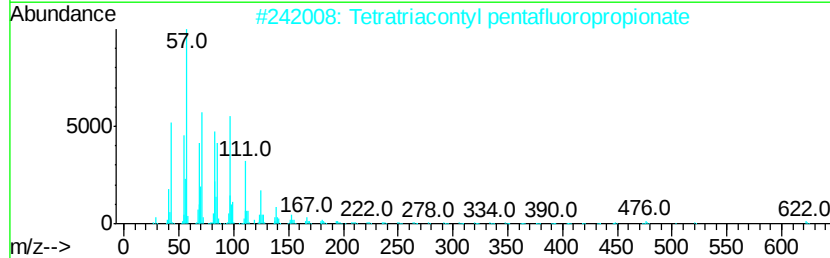
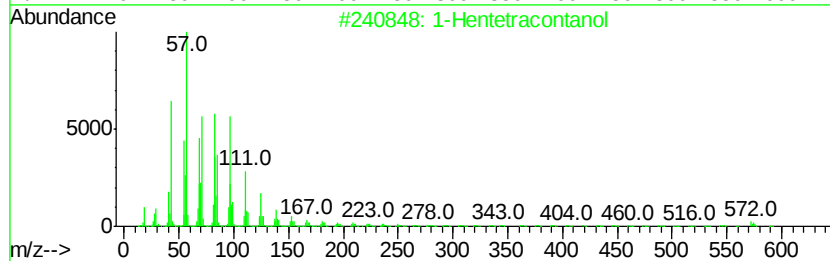
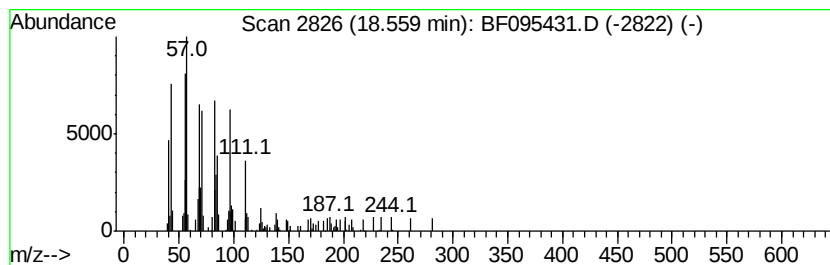
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Peak Number 6 1-Hentetracontanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.56	2.83 ng	80695	Chrysene-d12	18.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hentetracontanol	593 C41H84O	040710-42-7	83
2	Tetratriacontyl pentafluoropropi...	641 C37H69F5O2	1000351-81-5	83
3	Tricosyl pentafluoropropionate	486 C26H47F5O2	1000351-81-0	83
4	Hexacosyl trifluoroacetate	478 C28H53F3O2	1000351-75-0	83
5	Hexatriacontyl pentafluoropropio...	669 C39H73F5O2	1000351-89-0	83



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SB-25COMP

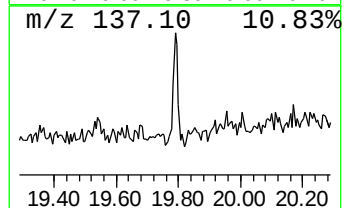
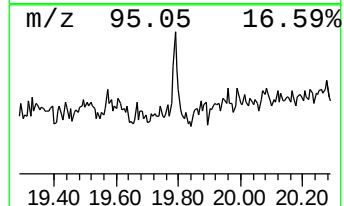
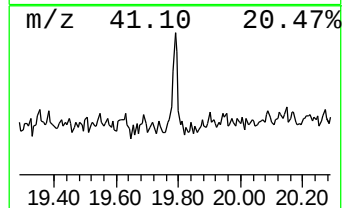
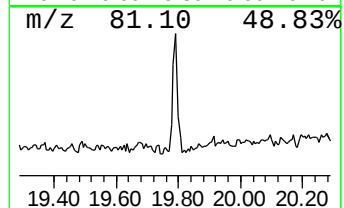
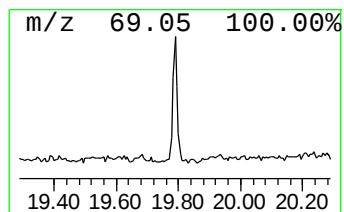
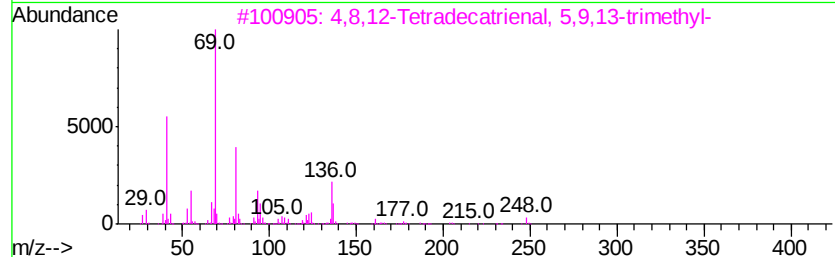
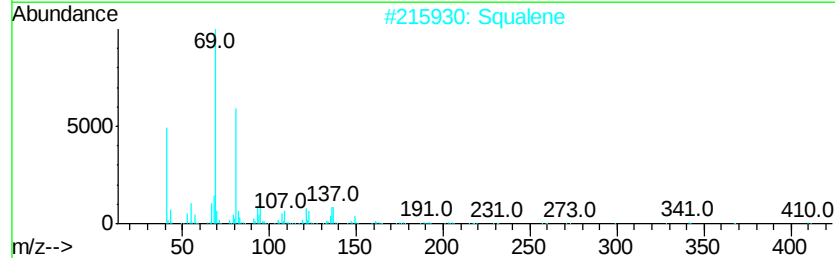
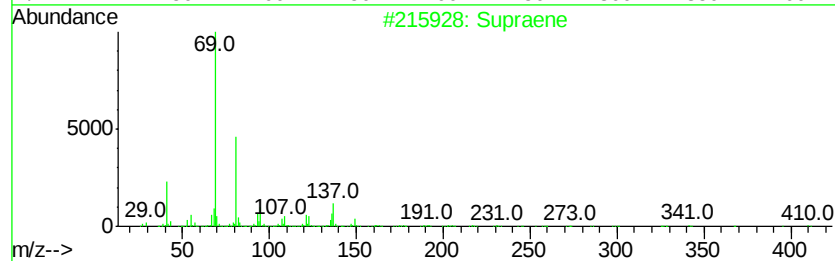
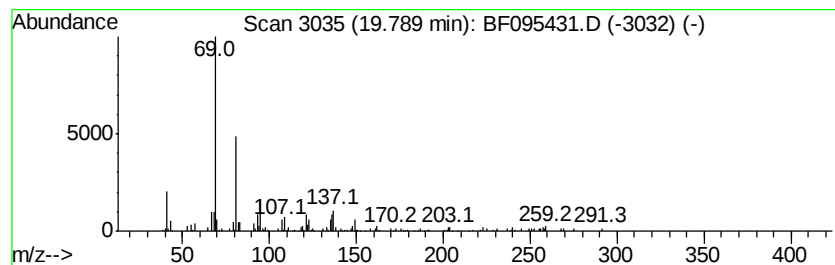
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.79	3.56 ng	84850	Perylene-d12	20.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	87
2		Squalene	410	C30H50	000111-02-4	80
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	56



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052517\
Data File : BF095431.D
Acq On : 25 May 2017 19:19
Operator : SJ/MA
Sample : I3332-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-25COMP

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	6.2	ng	176241	1	7.74	566392	20.0
unknown7.41	7.41	85.8	ng	2429650	1	7.74	566392	20.0
Decane, 1-iodo-	14.20	3.3	ng	127649	4	15.00	774107	20.0
n-Hexadecanoic acid	15.96	4.7	ng	181431	4	15.00	774107	20.0
1-Hentetracontanol	18.56	2.8	ng	80695	5	18.68	571225	20.0
Supraene	19.79	3.6	ng	84850	6	20.35	476298	20.0