

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
 Data File : BF102865.D
 Acq On : 8 Feb 2018 19:22
 Operator : SJ/JU
 Sample : J1470-15
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-12

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-BF020318.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	2.146	6	10	30	rVB	416447	630987	21.40%	2.380%
2	5.075	502	508	511	rBV	27642	31886	1.08%	0.120%
3	5.104	511	513	524	rVB	74776	87589	2.97%	0.330%
4	5.498	576	580	584	rBV	3211828	2949054	100.00%	11.122%
5	6.510	747	752	755	rBV	3095101	2882029	97.73%	10.869%
6	6.651	772	776	780	rBV	3101121	2934025	99.49%	11.065%
7	6.887	812	816	819	rBV	1350299	1138432	38.60%	4.293%
8	7.040	838	842	846	rBV	2253054	1934776	65.61%	7.297%
9	7.445	906	911	914	rBV	2160371	1797338	60.95%	6.778%
10	7.628	938	942	947	rVB	37049	33609	1.14%	0.127%
11	8.169	1030	1034	1037	rBV	1713321	1384242	46.94%	5.221%
12	9.239	1212	1216	1226	rBV	2477791	2165736	73.44%	8.168%
13	9.316	1226	1229	1232	rVB	87147	65858	2.23%	0.248%
14	9.633	1279	1283	1286	rBV	275349	244786	8.30%	0.923%
15	9.845	1316	1319	1323	rVB	195806	151602	5.14%	0.572%
16	9.922	1329	1332	1341	rVB	1362410	1268126	43.00%	4.783%
17	10.169	1371	1374	1378	rBV3	34573	34279	1.16%	0.129%
18	10.322	1397	1400	1402	rBV	54939	48402	1.64%	0.183%
19	10.345	1402	1404	1407	rVB	190449	142614	4.84%	0.538%
20	10.563	1437	1441	1444	rBV	46003	56237	1.91%	0.212%
21	10.710	1463	1466	1476	rVB	1249968	1168115	39.61%	4.405%
22	10.822	1482	1485	1493	rVB	140779	164181	5.57%	0.619%
23	11.269	1558	1561	1563	rBV	88711	71830	2.44%	0.271%
24	11.410	1581	1585	1589	rBV	1058232	978284	33.17%	3.690%
25	11.692	1631	1633	1636	rBV	48518	42104	1.43%	0.159%
26	12.810	1820	1823	1826	rBV	57936	49270	1.67%	0.186%
27	12.992	1850	1854	1858	rBV	1622175	1406211	47.68%	5.303%
28	13.468	1931	1935	1941	rBV	185522	216535	7.34%	0.817%
29	13.880	2001	2005	2014	rBV	341404	362354	12.29%	1.367%
30	14.051	2031	2034	2041	rVB	1011146	965150	32.73%	3.640%
31	14.804	2159	2162	2170	rBV3	126722	192913	6.54%	0.728%
32	14.898	2175	2178	2184	rVB	47635	58116	1.97%	0.219%
33	15.539	2282	2287	2295	rBV	621297	858647	29.12%	3.238%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

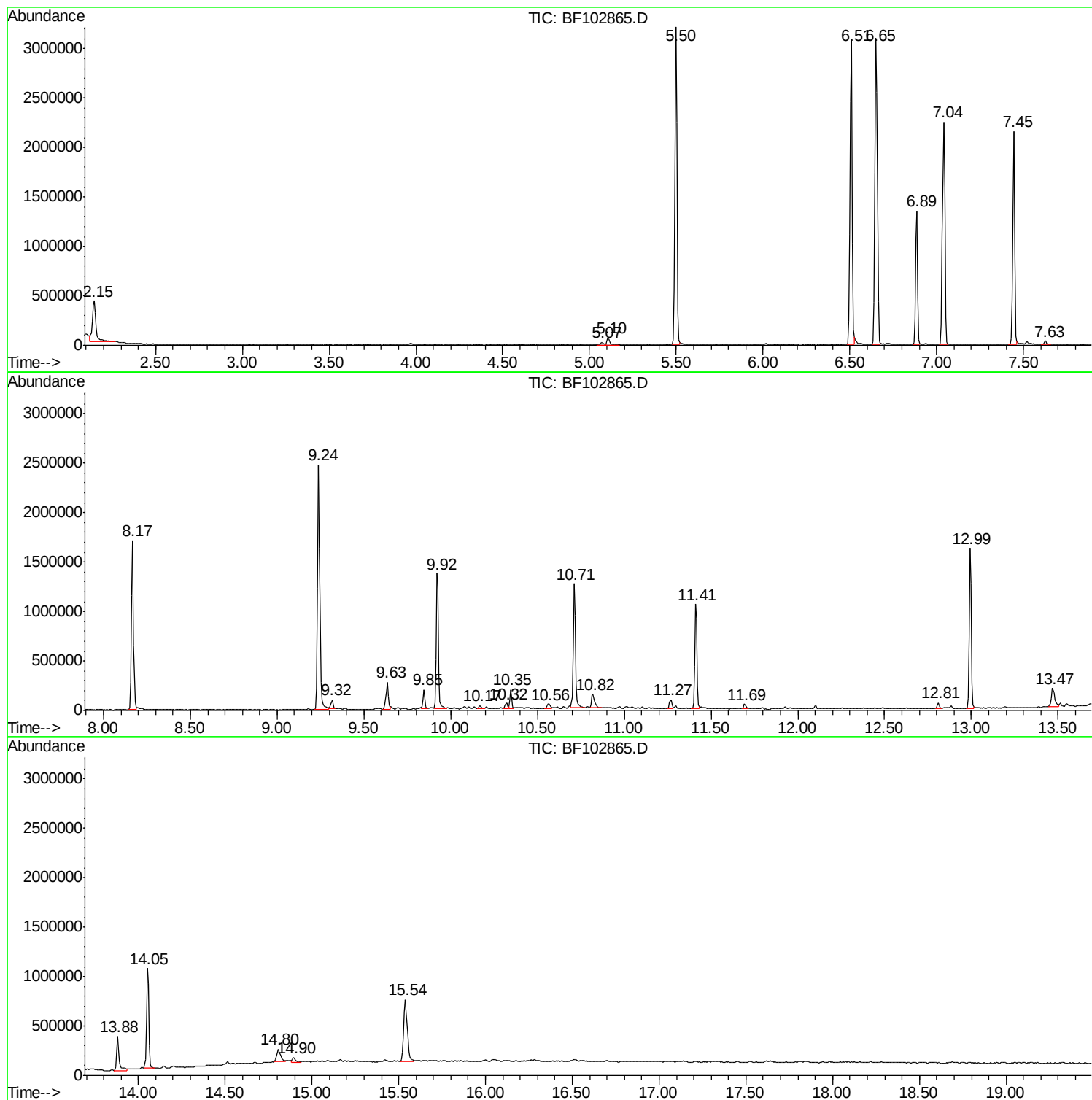
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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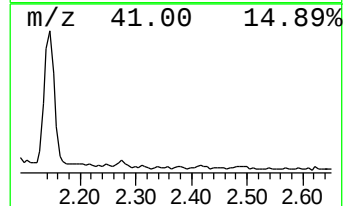
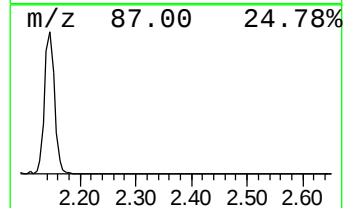
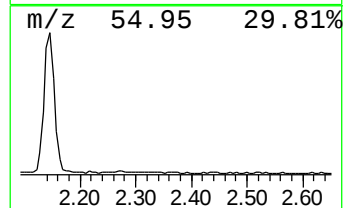
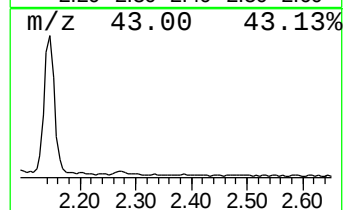
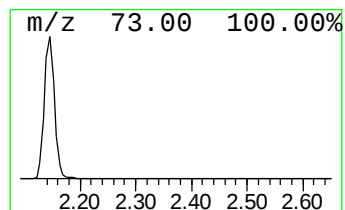
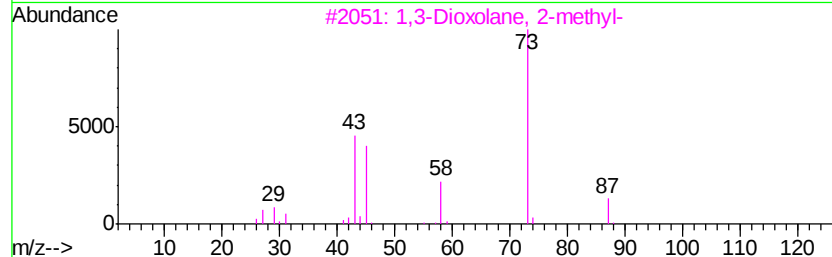
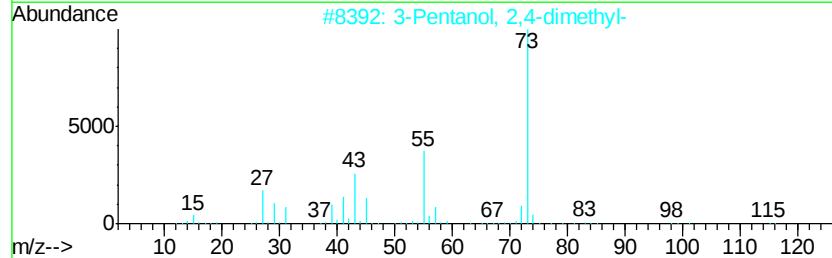
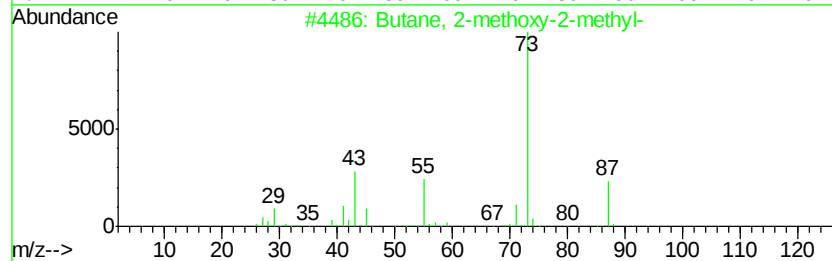
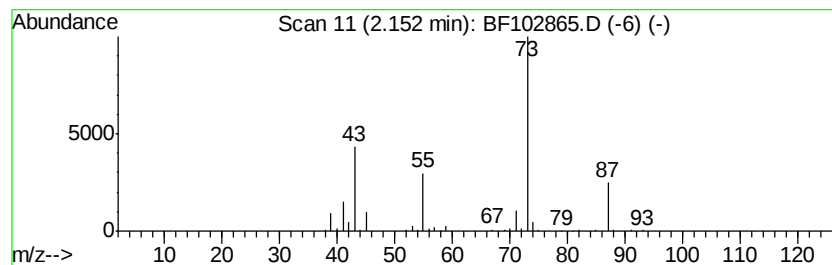
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	11.09 ng	630987	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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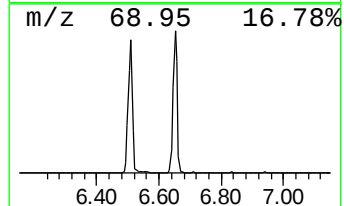
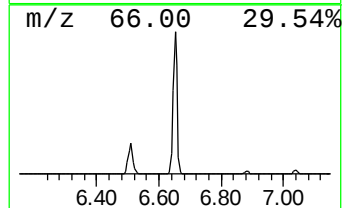
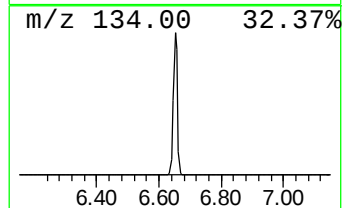
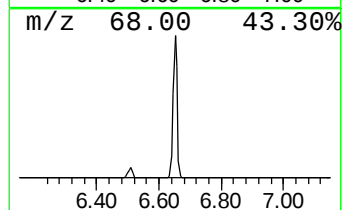
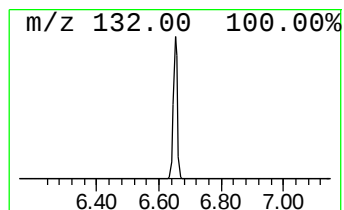
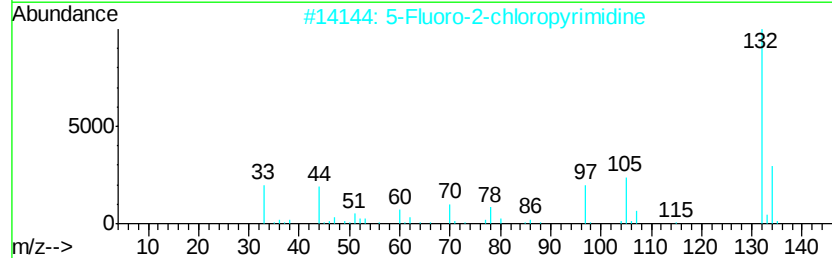
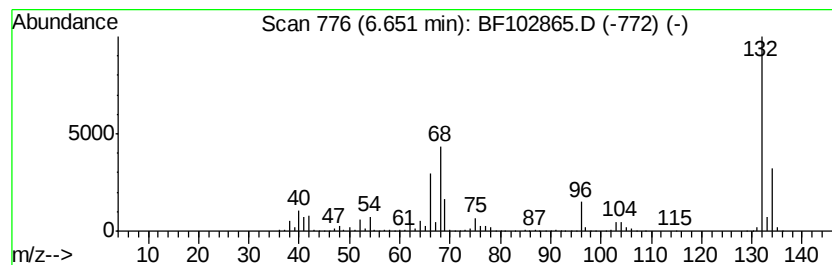
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	51.55 ng	2934030	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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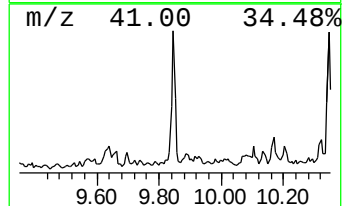
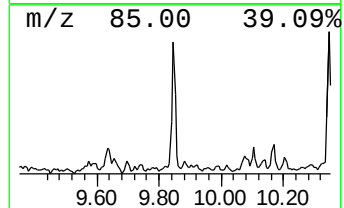
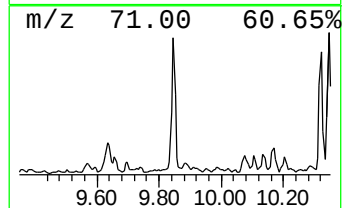
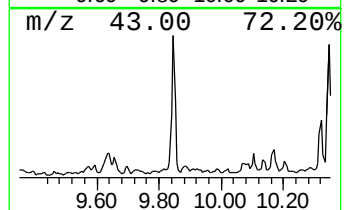
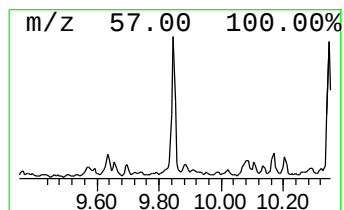
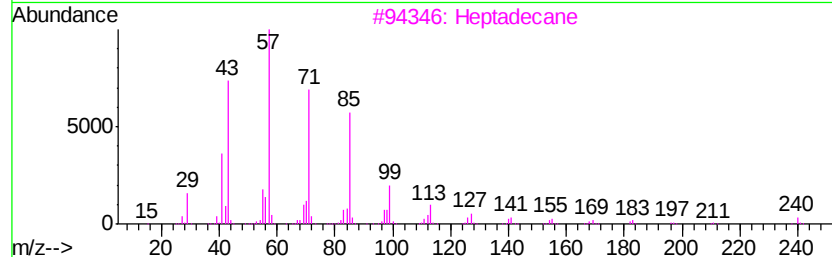
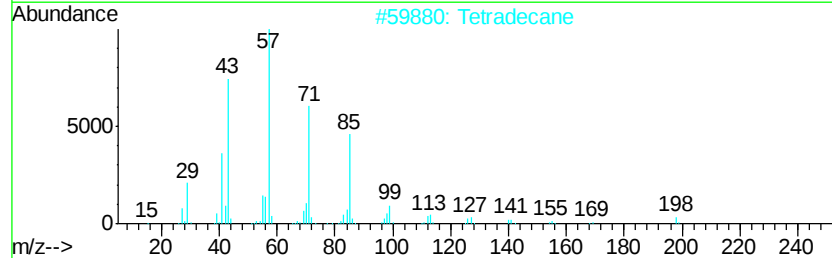
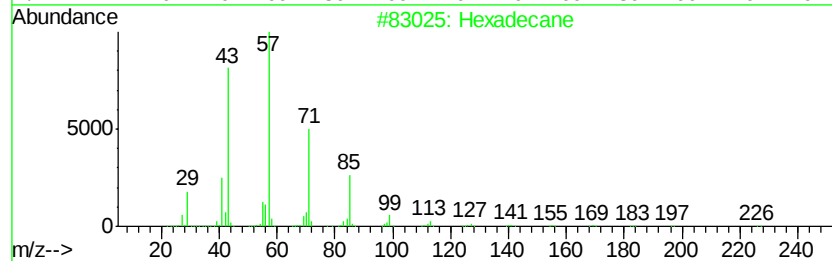
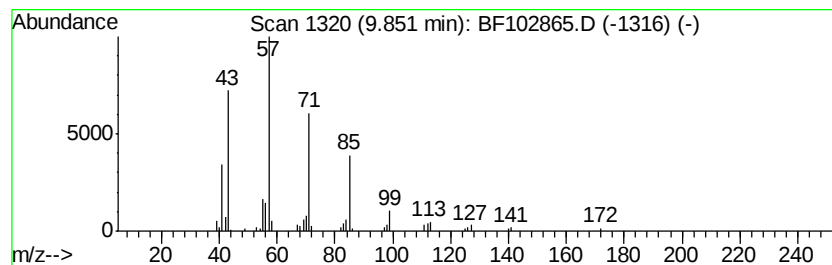
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.85	2.39 ng	151602	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	91
2	Tetradecane	198 C14H30	000629-59-4	86
3	Heptadecane	240 C17H36	000629-78-7	83
4	Tridecane	184 C13H28	000629-50-5	83
5	Sulfurous acid, hexyl pentyl ester	236 C11H24O3S	1000309-14-1	64



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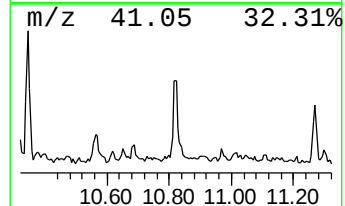
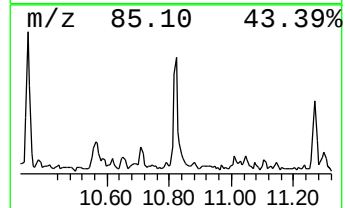
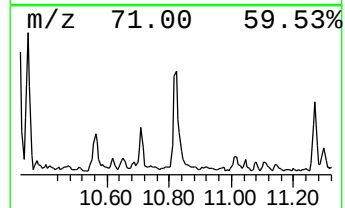
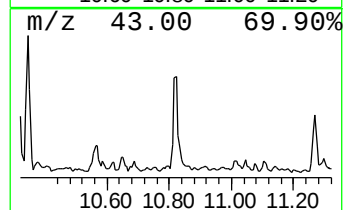
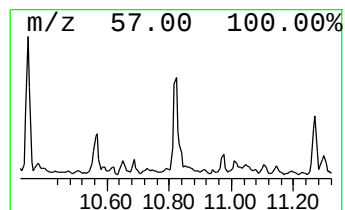
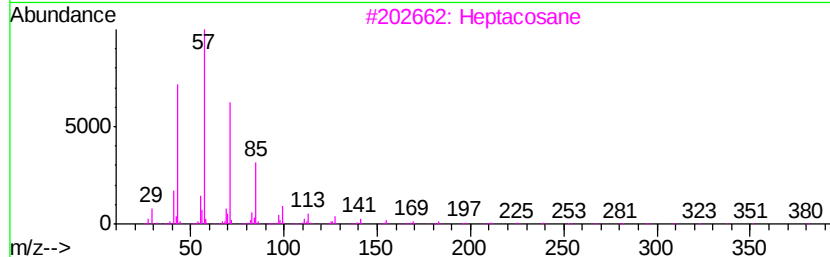
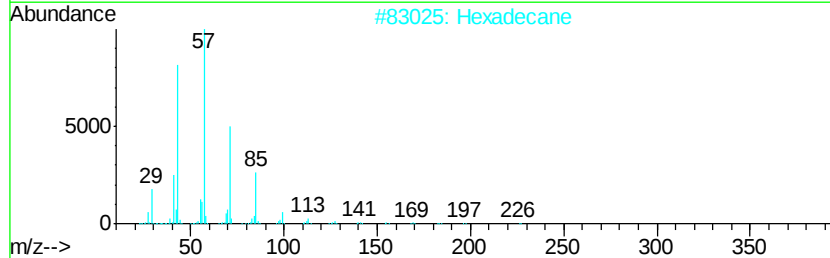
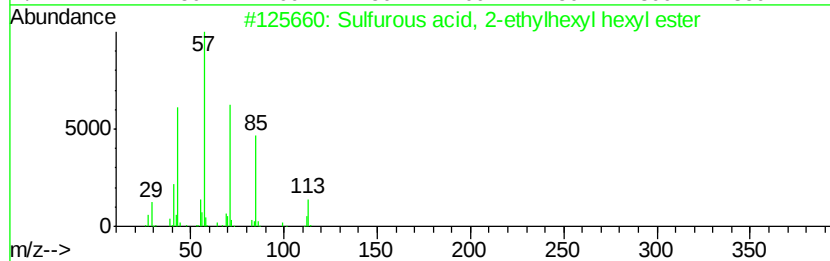
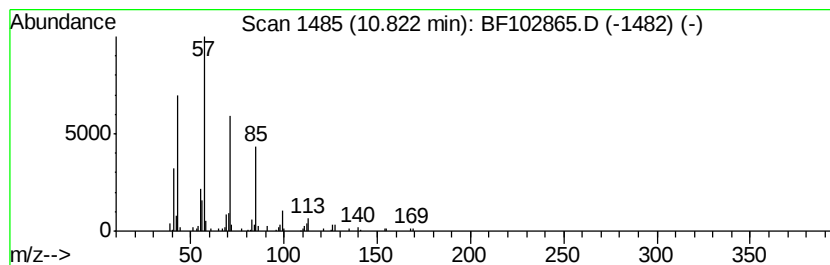
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Sulfurous acid, 2-ethylhexy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.82	3.36 ng	164181	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
2		Hexadecane	226	C16H34	000544-76-3	72
3		Heptacosane	380	C27H56	000593-49-7	64
4		Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	64
5		Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64



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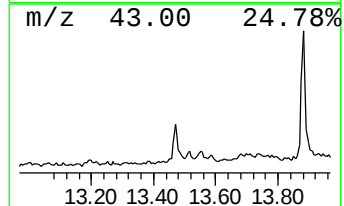
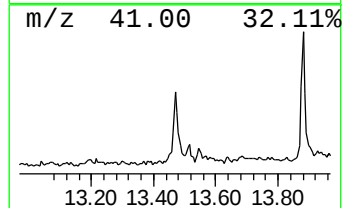
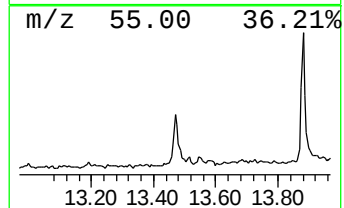
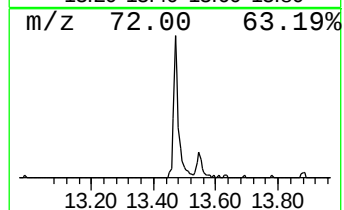
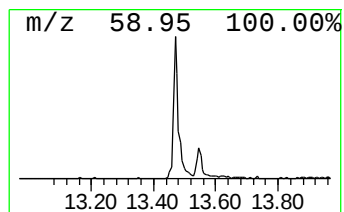
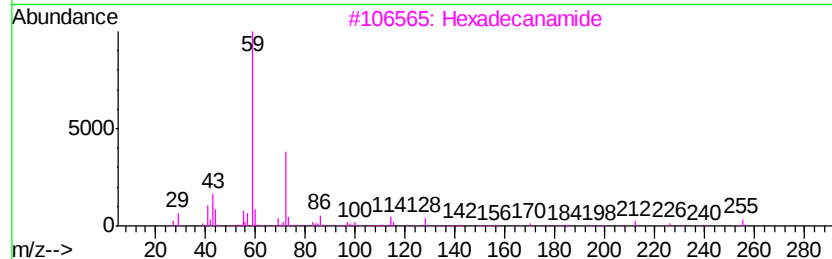
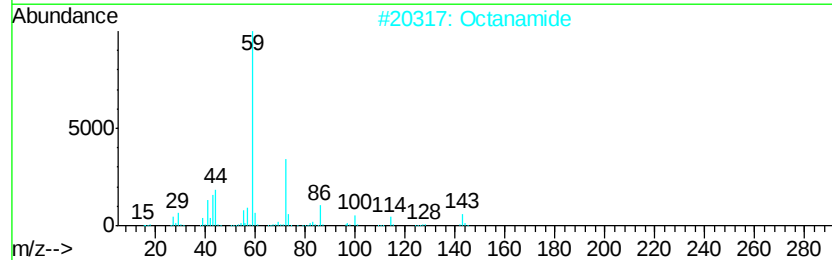
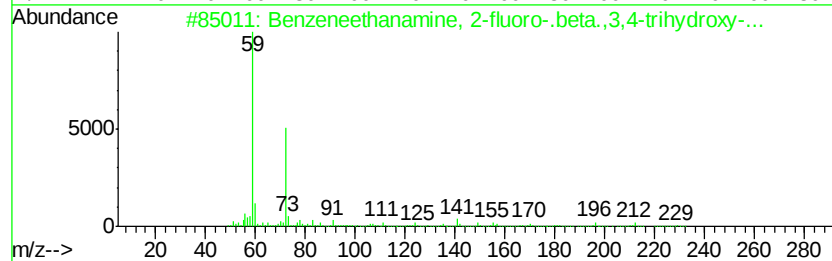
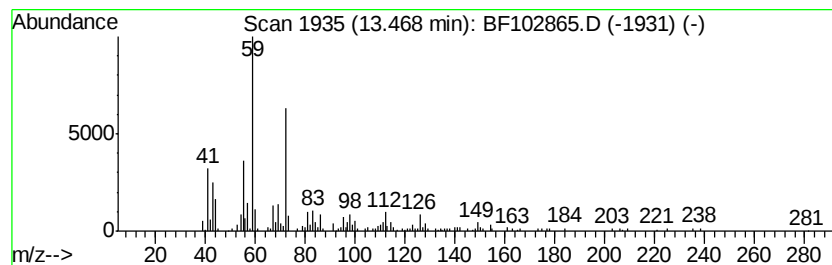
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzeneethanamine, 2-fluoro... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.49 ng	216535	Chrysene-d12	14.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
2		Octanamide	143	C8H17NO	000629-01-6	53
3		Hexadecanamide	255	C16H33NO	000629-54-9	53
4		Decanamide-	171	C10H21NO	002319-29-1	50
5		Nonanamide	157	C9H19NO	001120-07-6	50



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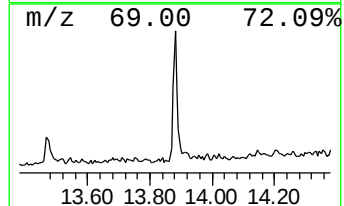
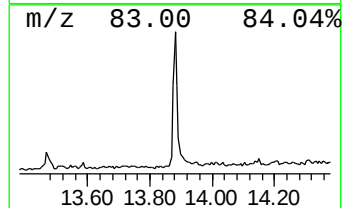
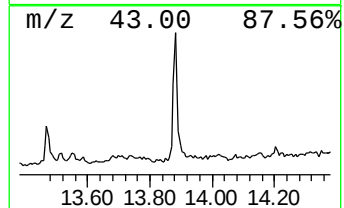
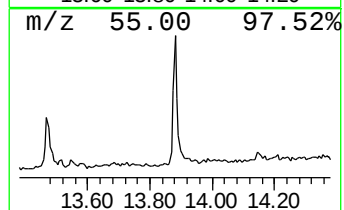
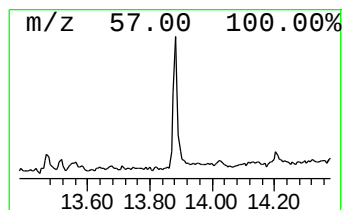
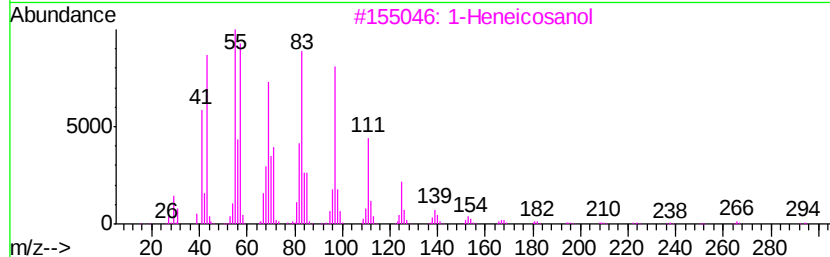
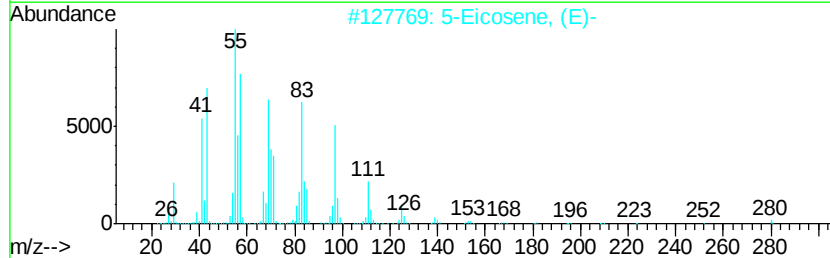
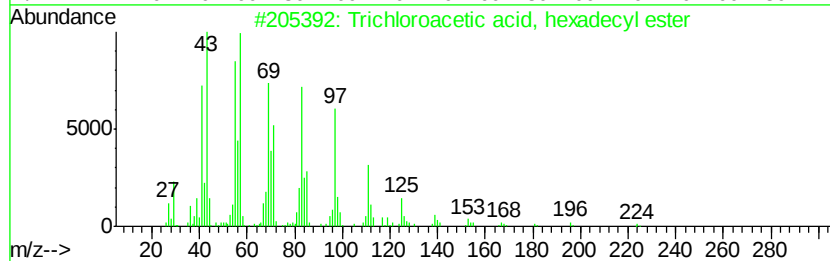
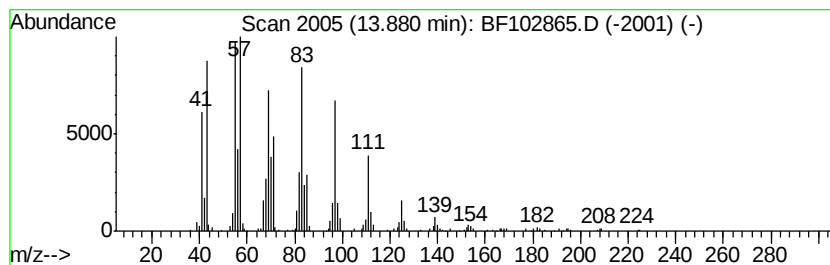
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.51 ng	362354	Chrysene-d12	14.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102865.D
Acq On : 8 Feb 2018 19:22
Operator : SJ/JU
Sample : J1470-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-12

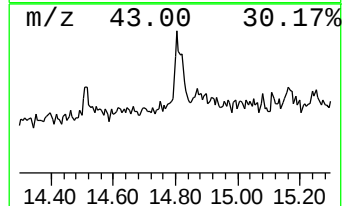
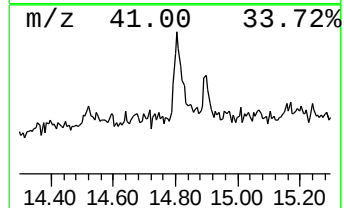
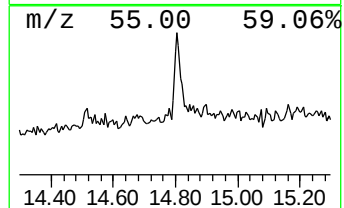
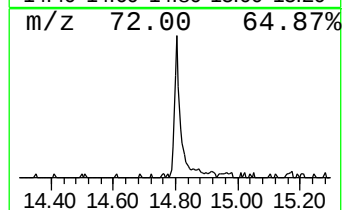
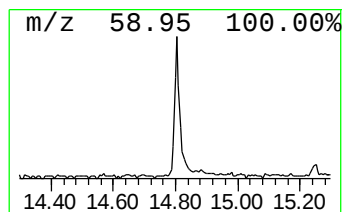
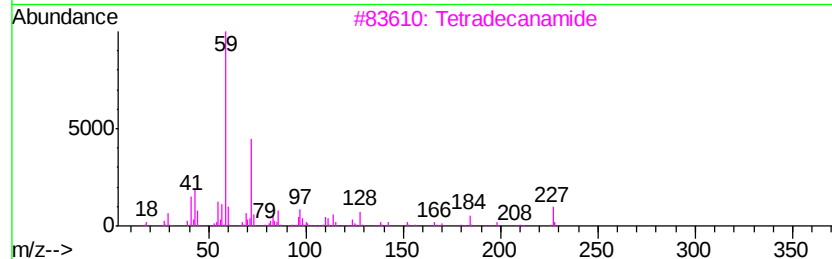
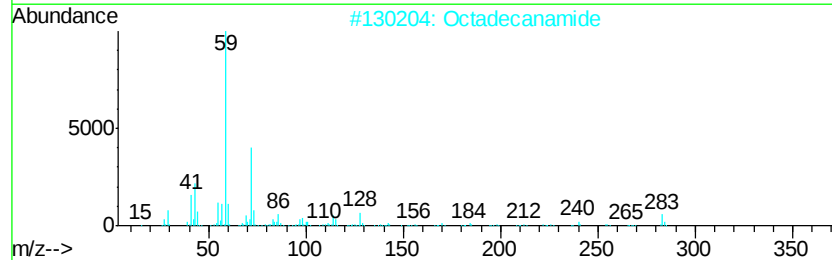
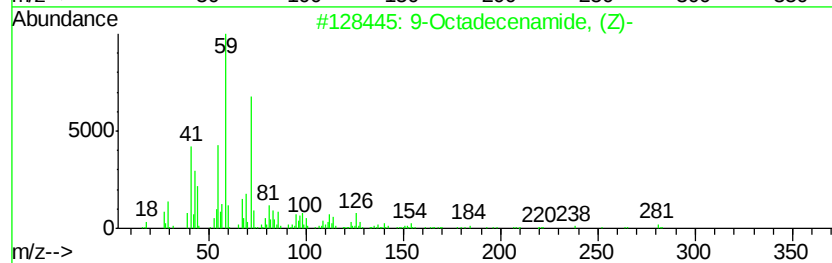
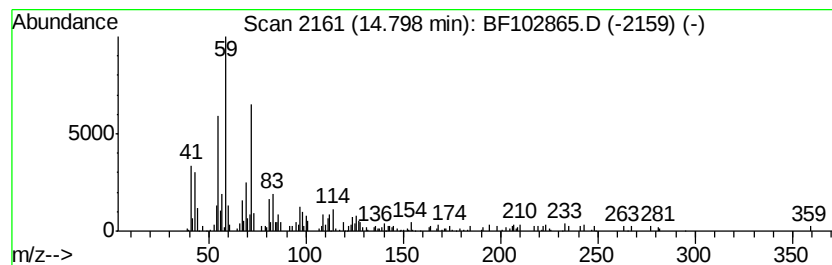
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.49 ng	192913	Perylene-d12	15.54

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	96
2		Octadecanamide	283	C18H37NO	000124-26-5	72
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Nonanamide	157	C9H19NO	001120-07-6	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102865.D
Acq On : 8 Feb 2018 19:22
Operator : SJ/JU
Sample : J1470-15
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-12

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
Butane, 2-methoxy...	2.15	11.1 ng		630987	1	6.89	1138430	20.0
unknown6.65	6.65	51.5 ng		2934030	1	6.89	1138430	20.0
Hexadecane	9.85	2.4 ng		151602	3	9.92	1268130	20.0
Sulfurous acid, 2...	10.82	3.4 ng		164181	4	11.41	978284	20.0
Benzeneethanamine...	13.47	4.5 ng		216535	5	14.05	965150	20.0
Trichloroacetic a...	13.88	7.5 ng		362354	5	14.05	965150	20.0
9-Octadecenamide,...	14.80	4.5 ng		192913	6	15.54	858647	20.0