

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
 Data File : BF109069.D
 Acq On : 18 Sep 2018 1:43
 Operator : JU/SJ
 Sample : J4936-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 138kv-2

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.266	323	328	337	rBV	551500	644158	21.03%	2.329%
2	4.913	434	438	450	rVB	688602	841988	27.48%	3.044%
3	5.337	504	510	513	rBV	2741971	2755888	89.96%	9.964%
4	6.360	678	684	687	rBV	2963220	2920741	95.34%	10.560%
5	6.490	702	706	709	rBV	3121963	2868333	93.63%	10.370%
6	6.719	742	745	749	rBV	926810	770318	25.14%	2.785%
7	6.878	768	772	775	rBV	2801045	2412072	78.73%	8.721%
8	7.278	835	840	844	rBV	1794089	1845627	60.24%	6.673%
9	8.001	959	963	966	rBV	1113316	861893	28.13%	3.116%
10	9.078	1142	1146	1149	rBV	3663371	3063565	100.00%	11.076%
11	9.466	1209	1212	1216	rBV	174956	153825	5.02%	0.556%
12	9.748	1257	1260	1264	rBV	954728	833591	27.21%	3.014%
13	10.536	1389	1394	1404	rBV	1611505	1567613	51.17%	5.668%
14	11.225	1508	1511	1515	rBV	944916	834725	27.25%	3.018%
15	12.813	1776	1781	1784	rBV	3320010	3003563	98.04%	10.859%
16	13.719	1929	1935	1947	rBV2	117519	207513	6.77%	0.750%
17	13.854	1954	1958	1961	rBV	1063413	949659	31.00%	3.433%
18	14.042	1987	1990	1998	rVB	31975	38572	1.26%	0.139%
19	14.342	2038	2041	2045	rBV	49671	46271	1.51%	0.167%
20	14.636	2088	2091	2099	rVB	61983	68311	2.23%	0.247%
21	14.954	2142	2145	2149	rVB	71299	68469	2.23%	0.248%
22	15.254	2191	2196	2202	rBV	543847	660370	21.56%	2.388%
23	15.307	2202	2205	2212	rVB	60957	79632	2.60%	0.288%
24	15.713	2270	2274	2280	rVB2	43195	62680	2.05%	0.227%
25	16.177	2350	2353	2358	rBV3	26192	37145	1.21%	0.134%
26	16.912	2474	2478	2486	rVB	31374	62506	2.04%	0.226%

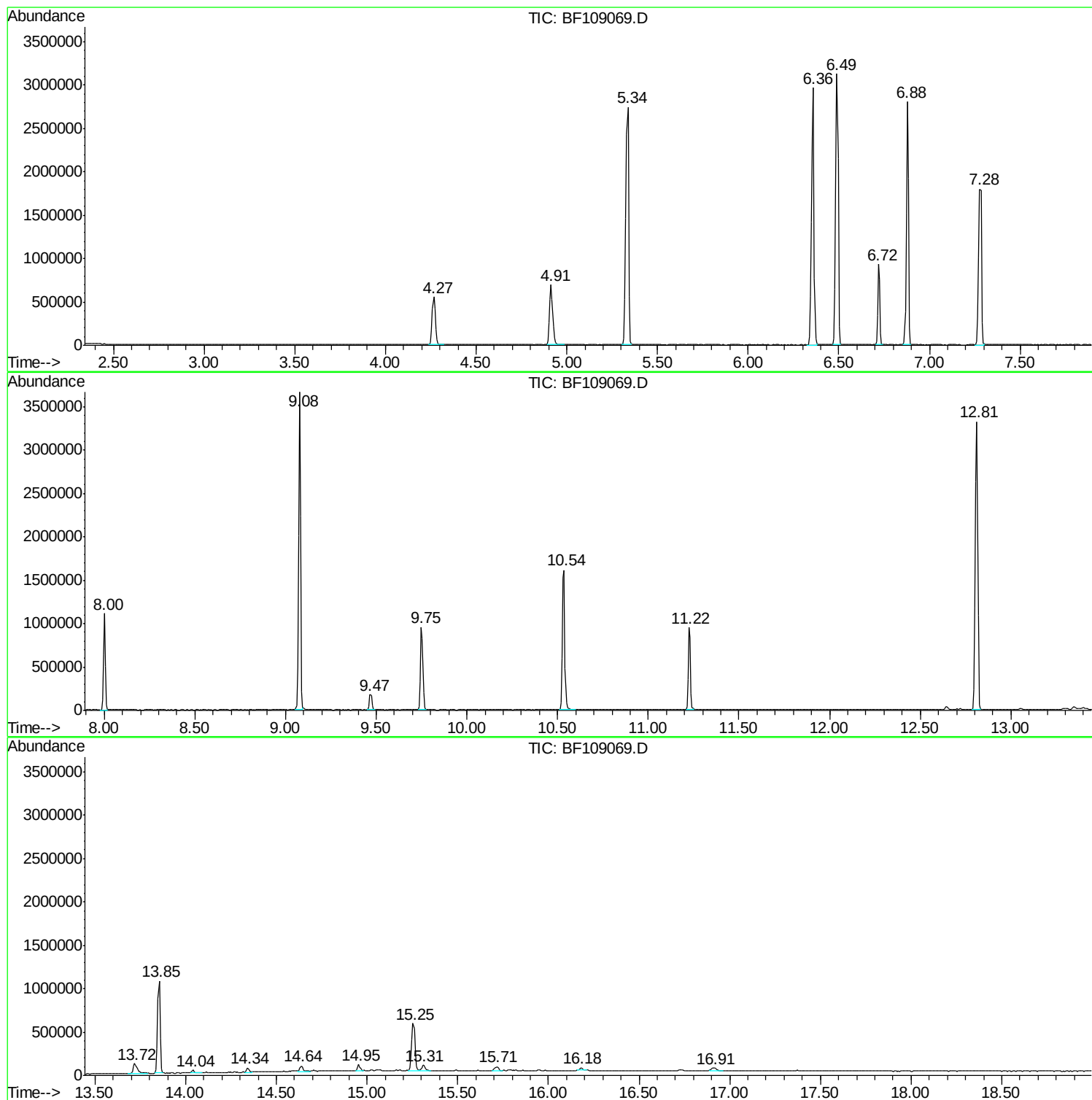
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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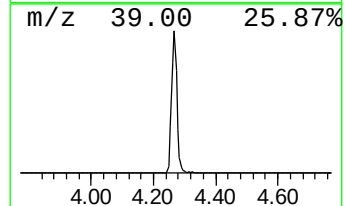
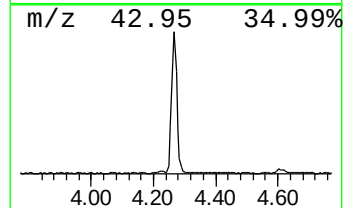
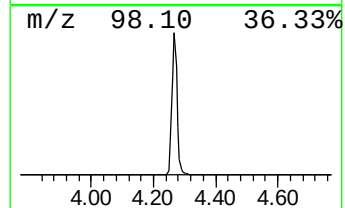
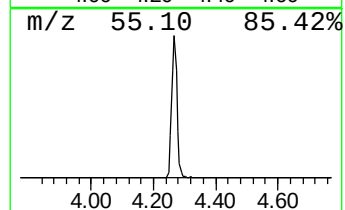
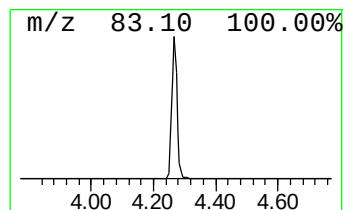
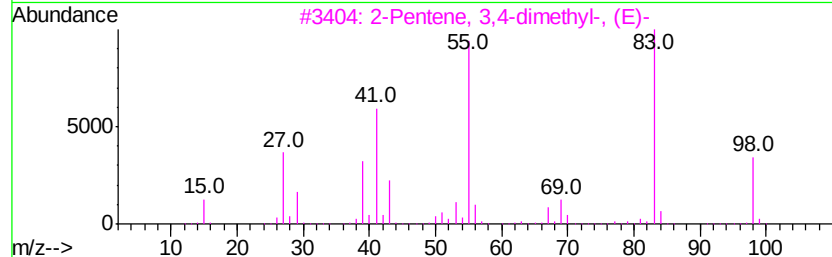
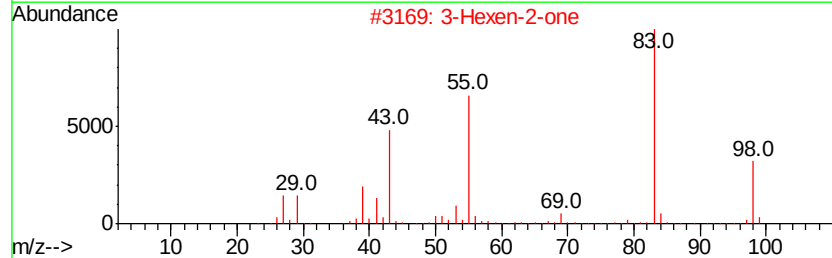
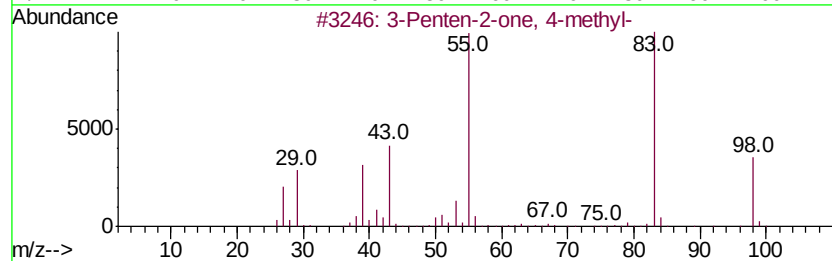
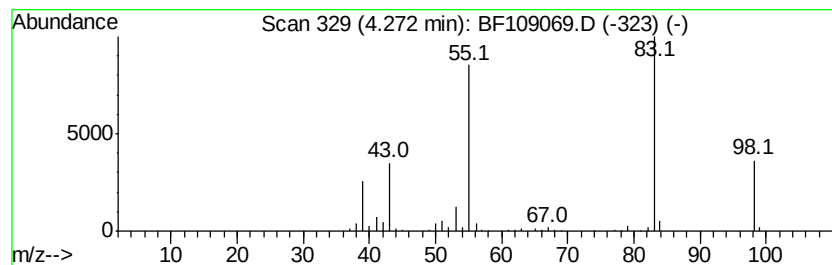
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	16.72 ng	644158	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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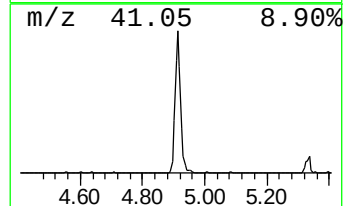
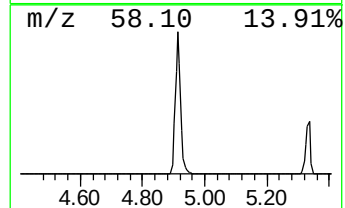
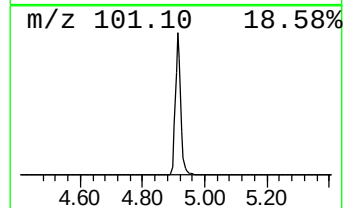
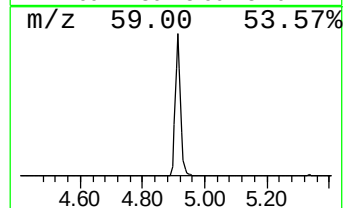
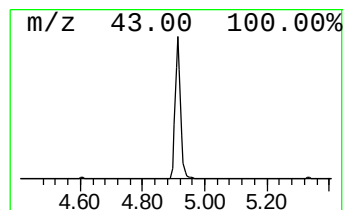
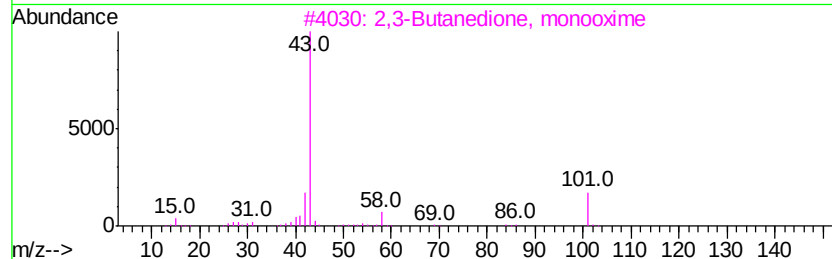
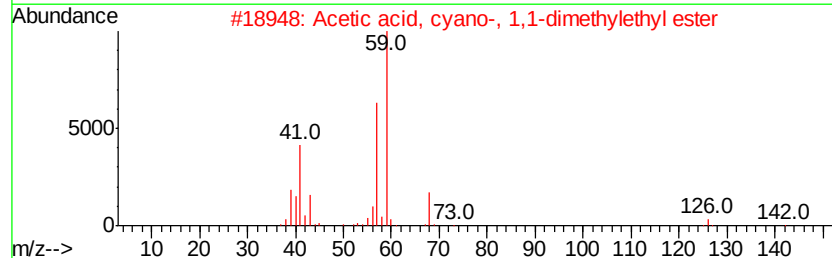
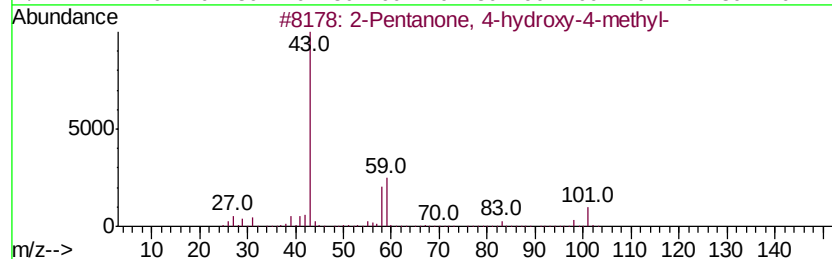
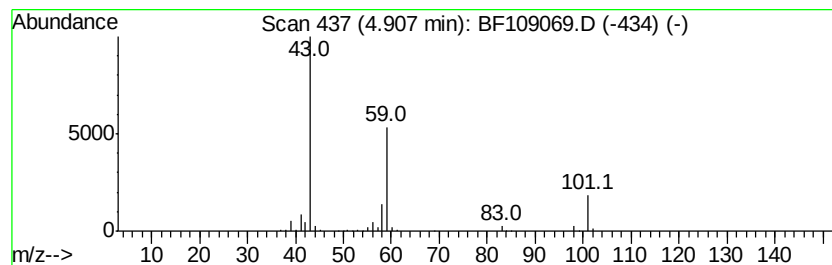
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	21.86 ng	841988	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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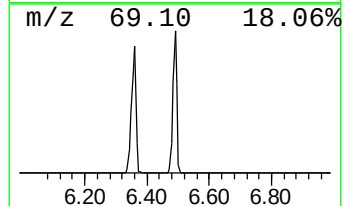
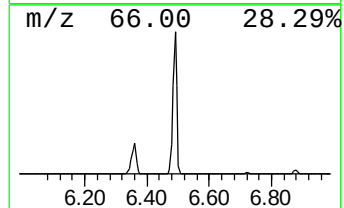
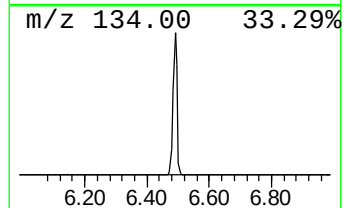
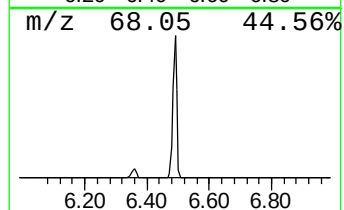
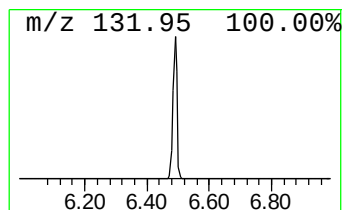
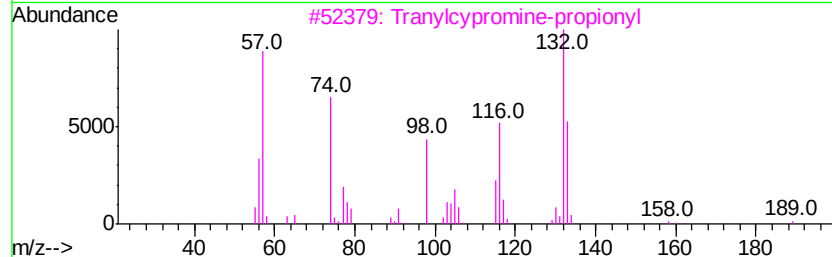
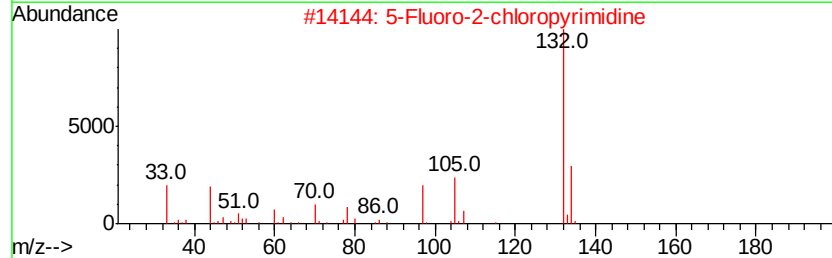
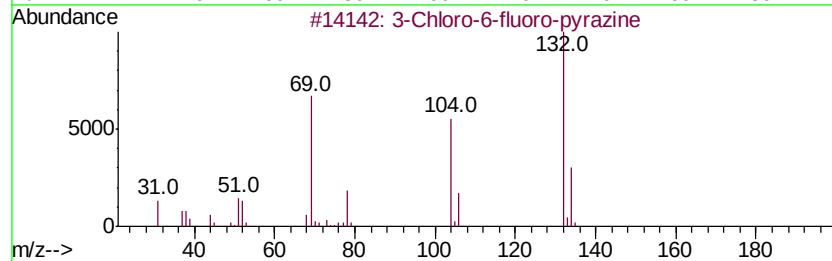
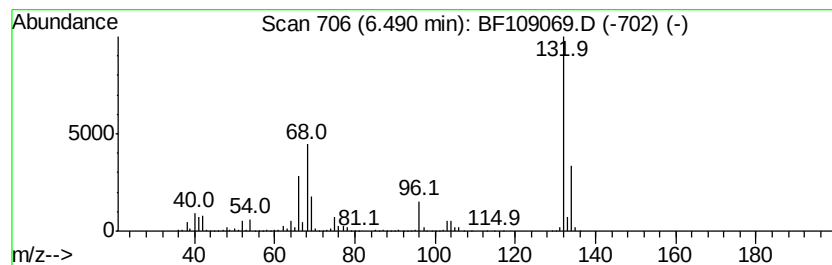
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Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	74.47 ng	2868330	1,4-Dichlorobenzene-d4	6.72

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		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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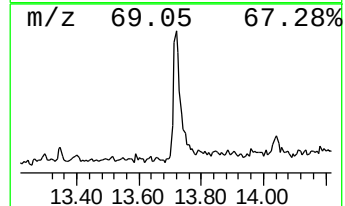
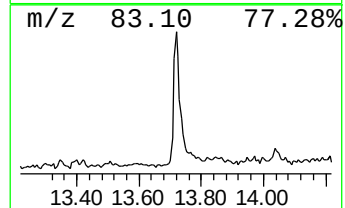
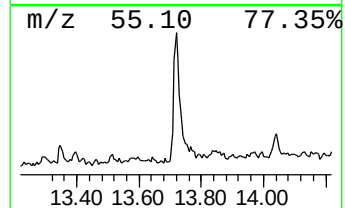
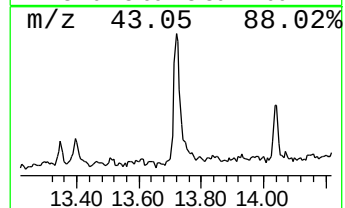
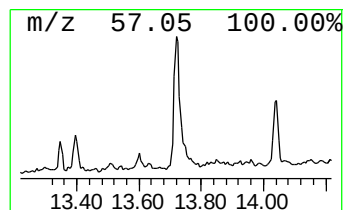
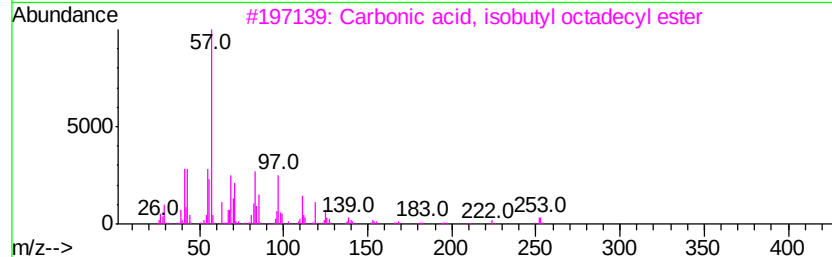
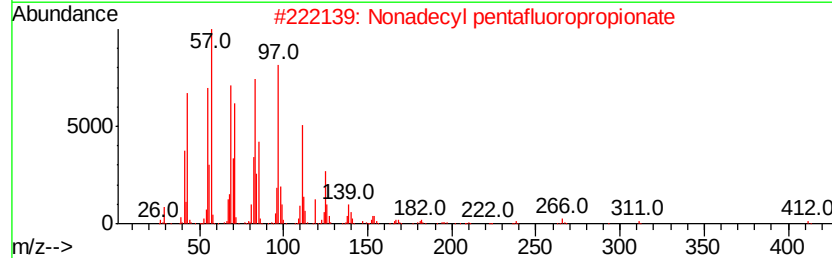
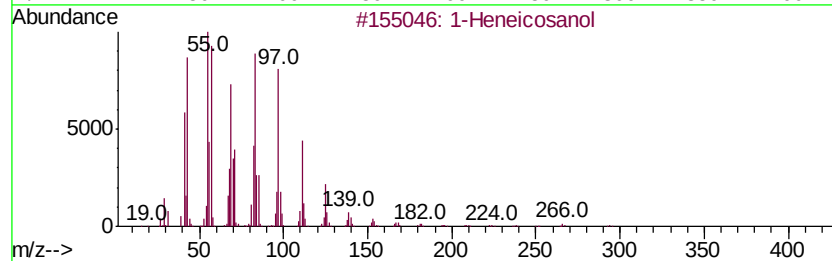
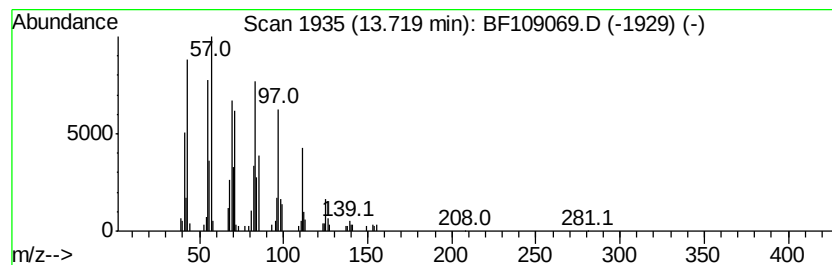
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.37 ng	207513	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	93
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3		Carbonic acid, isobutyl octadecyl...	370	C23H46O3	1000314-61-5	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5		1-Docosene	308	C22H44	001599-67-3	83



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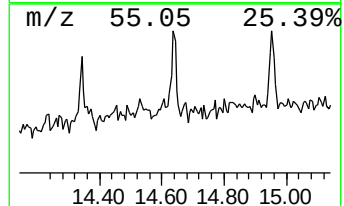
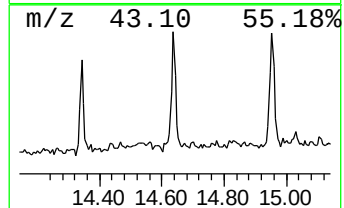
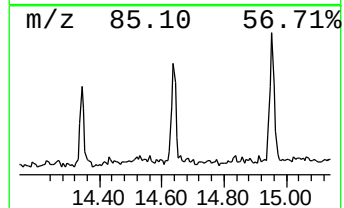
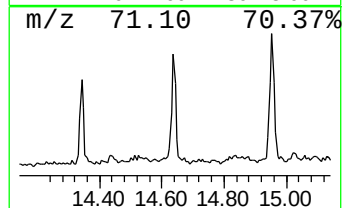
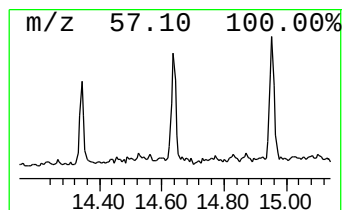
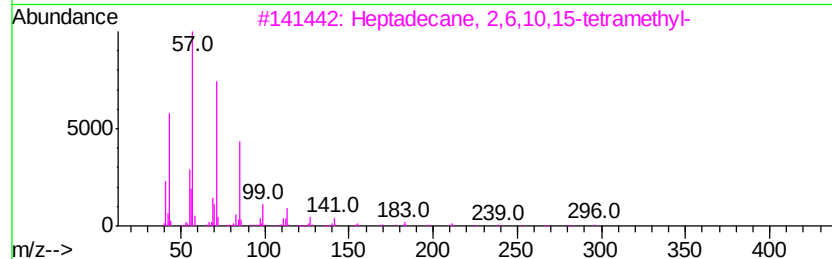
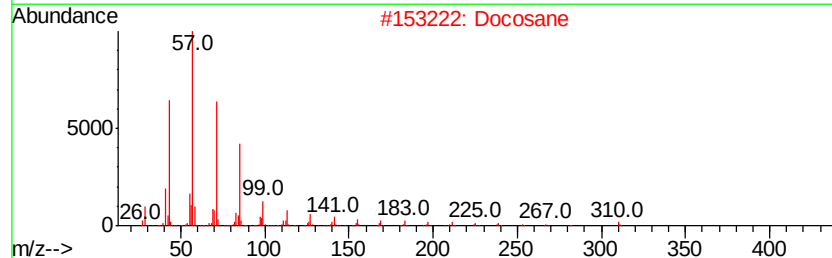
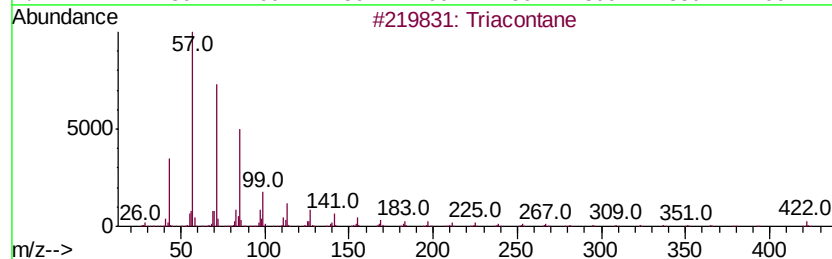
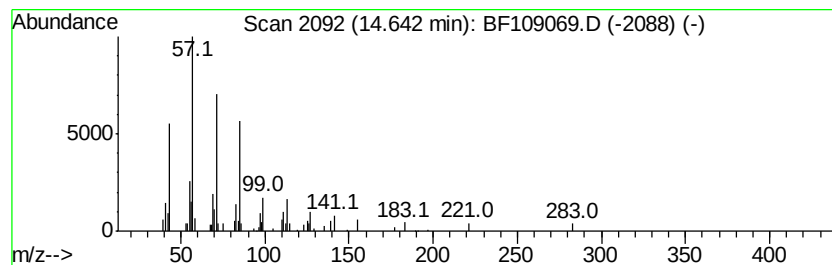
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.07 ng	68311	Perylene-d12	15.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Triacontane	422	C30H62	000638-68-6	91
2		Docosane	310	C22H46	000629-97-0	90
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4		Heptacosane	380	C27H56	000593-49-7	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



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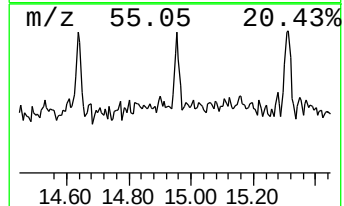
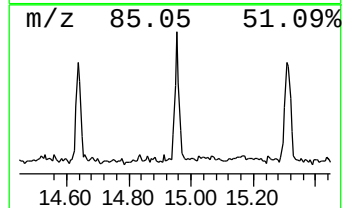
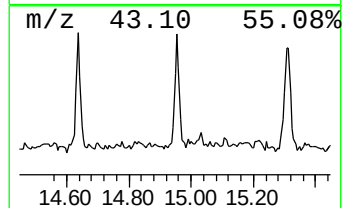
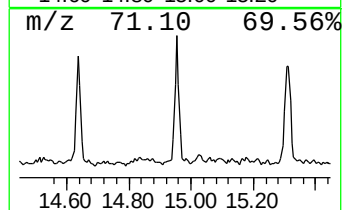
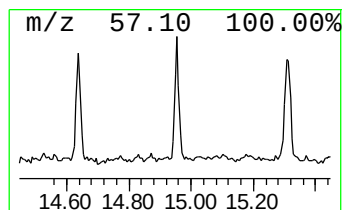
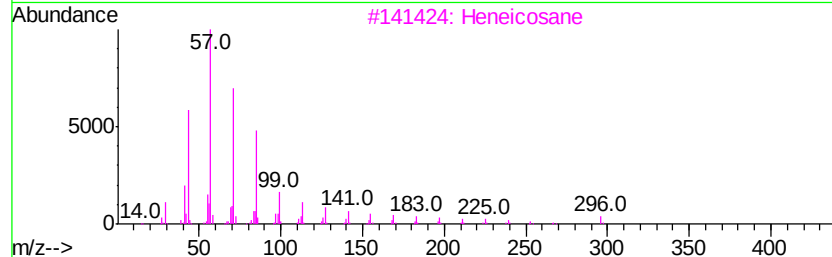
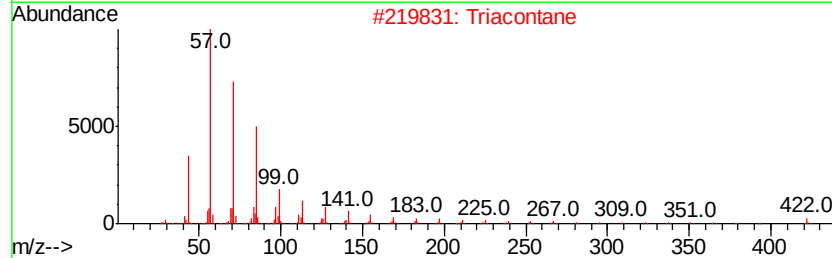
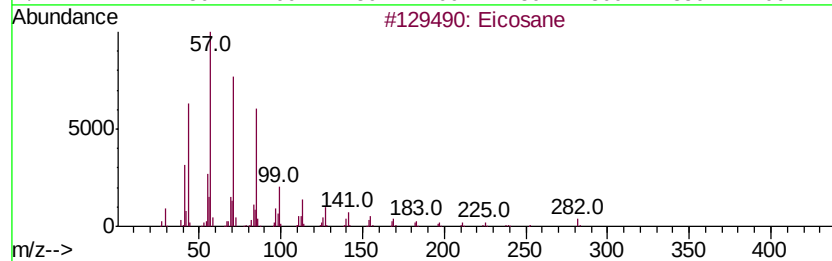
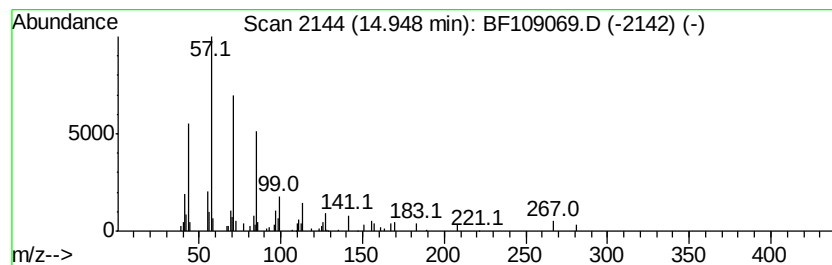
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.07 ng	68469	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	94
2		Triacotane	422	C30H62	000638-68-6	91
3		Heneicosane	296	C21H44	000629-94-7	91
4		Docosane	310	C22H46	000629-97-0	90
5		Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091718\
Data File : BF109069.D
Acq On : 18 Sep 2018 1:43
Operator : JU/SJ
Sample : J4936-03
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
138kv-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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
3-Penten-2-one, 4...	4.27	16.7	ng	644158	1	6.72	770318	20.0
2-Pentanone, 4-hy...	4.91	21.9	ng	841988	1	6.72	770318	20.0
unknown6.49	6.49	74.5	ng	2868330	1	6.72	770318	20.0
1-Heneicosanol	13.72	4.4	ng	207513	5	13.85	949659	20.0
Triacontane	14.64	2.1	ng	68311	6	15.25	660370	20.0
Eicosane	14.95	2.1	ng	68469	6	15.25	660370	20.0