

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121018\
 Data File : BF111261.D
 Acq On : 10 Dec 2018 23:59
 Operator : JU/SJ
 Sample : J6306-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VB-16204

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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	2.487	65	68	74	rVB	87765	139690	1.06%	0.147%
2	3.263	198	200	216	rBV4	89011	218964	1.65%	0.231%
3	4.663	433	438	442	rBV	133754	142081	1.07%	0.150%
4	5.028	496	500	507	rVB	470592	663474	5.01%	0.698%
5	5.175	521	525	541	rBV	1533396	1716595	12.97%	1.807%
6	5.287	541	544	550	rVB	142461	138663	1.05%	0.146%
7	5.428	557	568	571	rBV	10324357	11216125	84.72%	11.808%
8	5.640	600	604	612	rVB3	213561	294538	2.22%	0.310%
9	6.334	718	722	725	rBV	245437	223275	1.69%	0.235%
10	6.440	732	740	747	rBV	10735574	13238510	100.00%	13.937%
11	6.492	747	749	758	rVV	228063	205496	1.55%	0.216%
12	6.575	758	763	766	rVV	11494192	11846827	89.49%	12.472%
13	6.634	770	773	778	rVB	392674	339617	2.57%	0.358%
14	6.804	798	802	805	rBV	2828500	2511970	18.97%	2.644%
15	6.963	824	829	832	rBV	8680969	8245881	62.29%	8.681%
16	7.363	891	897	900	rBV	7423749	7506403	56.70%	7.902%
17	7.957	991	998	1001	rBV	168815	183468	1.39%	0.193%
18	8.081	1015	1019	1023	rBV	2866840	2571805	19.43%	2.707%
19	9.163	1197	1203	1206	rBV	11328297	10017240	75.67%	10.546%
20	9.551	1266	1269	1272	rBV	1261602	948634	7.17%	0.999%
21	9.839	1311	1318	1321	rBV	2820476	2455361	18.55%	2.585%
22	10.622	1447	1451	1455	rBV	5440022	5255600	39.70%	5.533%
23	11.063	1523	1526	1534	rVB	360876	459409	3.47%	0.484%
24	11.322	1566	1570	1573	rBV	2321676	2158304	16.30%	2.272%
25	11.857	1657	1661	1668	rBV	952734	978357	7.39%	1.030%
26	11.910	1668	1670	1676	rVB3	116871	181794	1.37%	0.191%
27	12.533	1772	1776	1778	rBV	152551	181672	1.37%	0.191%
28	12.639	1791	1794	1799	rBV	420554	451151	3.41%	0.475%
29	12.692	1799	1803	1807	rVB2	159516	233809	1.77%	0.246%
30	12.910	1835	1840	1843	rBV	6706102	6156168	46.50%	6.481%
31	13.957	2014	2018	2021	rBV	2392269	2246856	16.97%	2.365%
32	15.392	2258	2262	2268	rBV	1377564	1631847	12.33%	1.718%
33	18.098	2718	2722	2724	rBV3	160047	230187	1.74%	0.242%

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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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

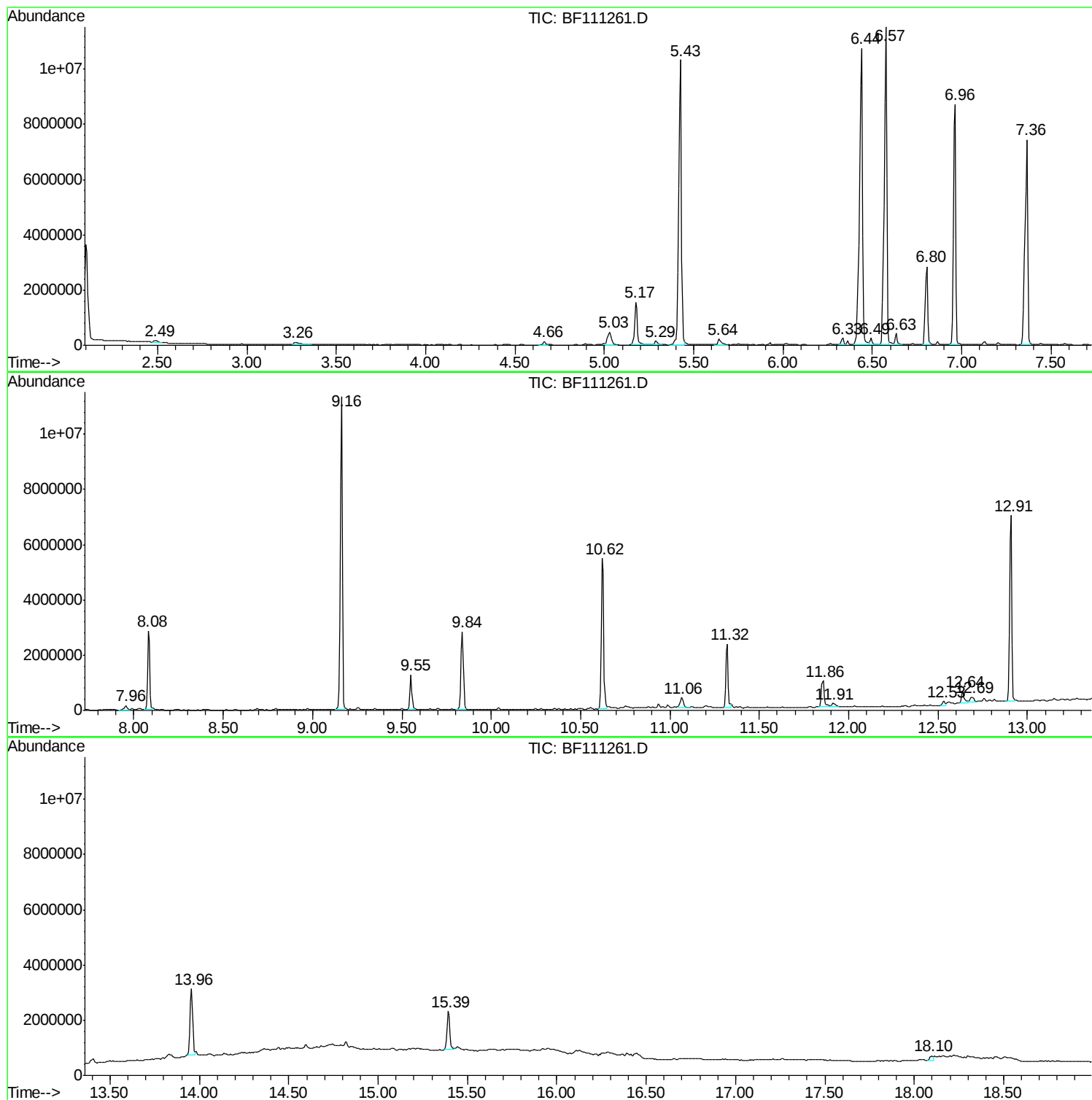
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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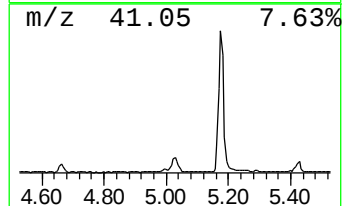
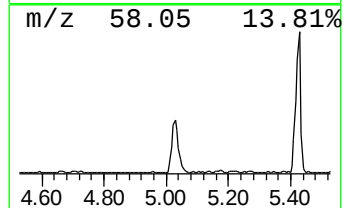
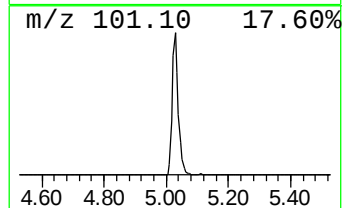
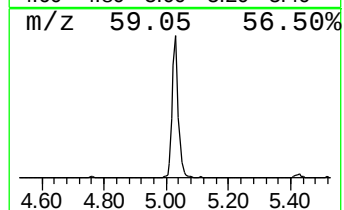
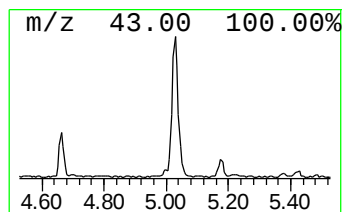
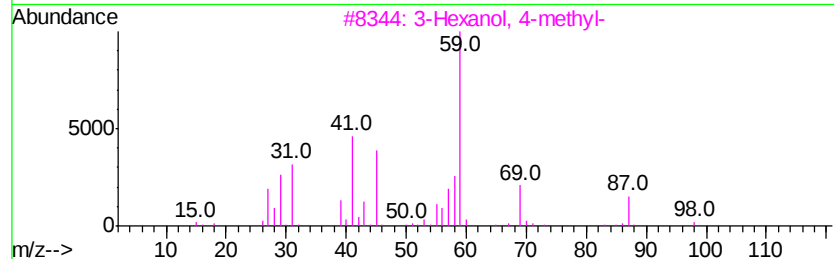
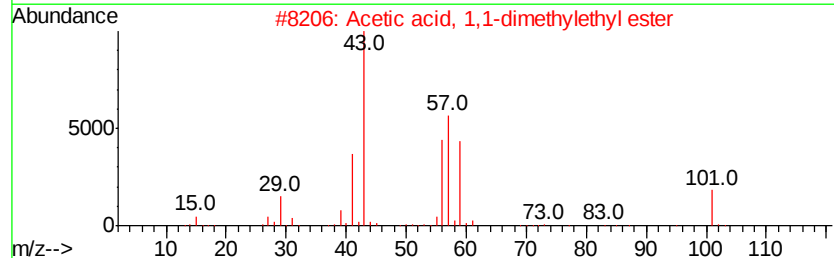
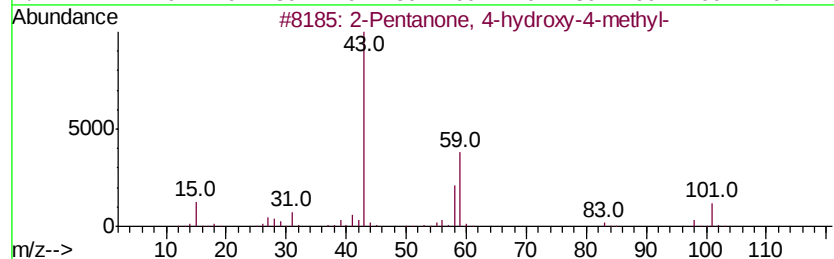
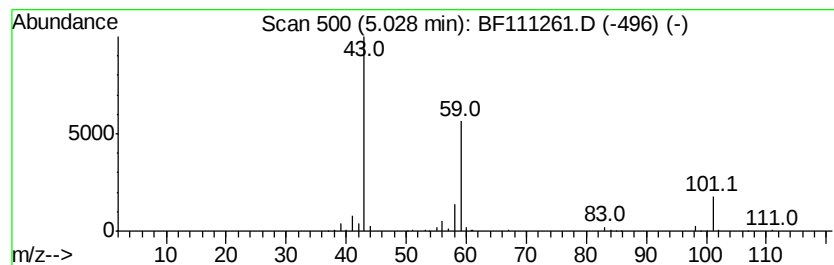
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.03	5.28 ng	663474	1,4-Dichlorobenzene-d4	6.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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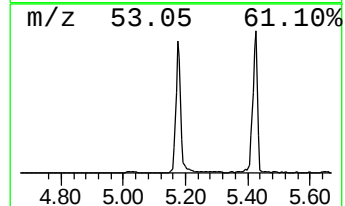
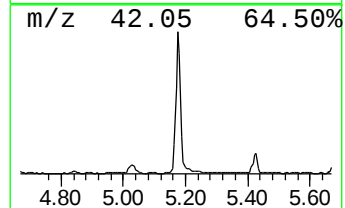
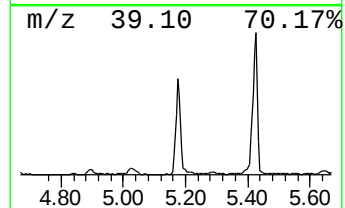
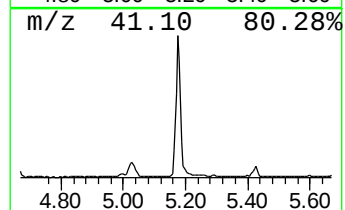
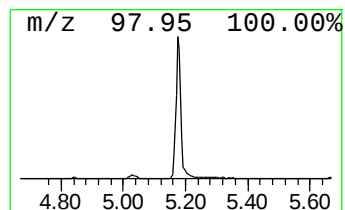
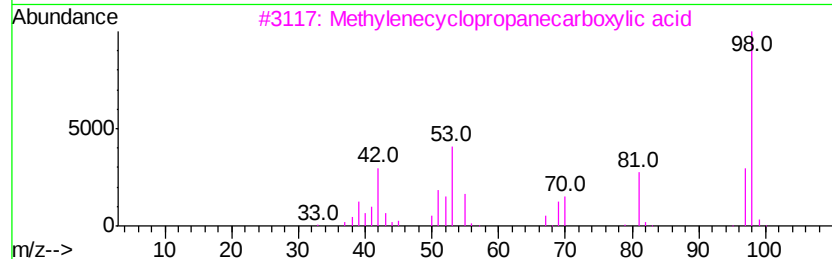
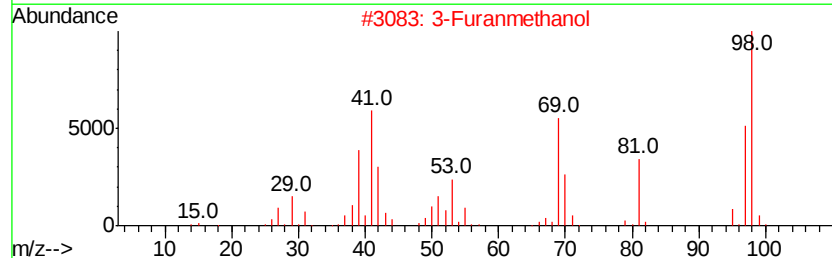
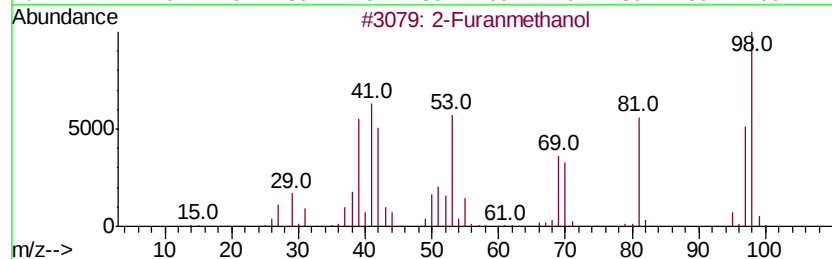
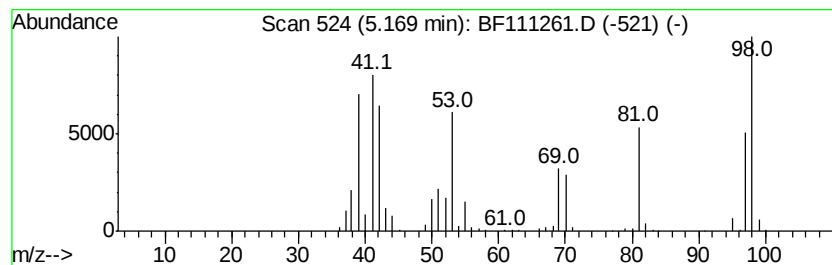
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Furanmethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	13.67 ng	1716600	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furanmethanol	98	C5H6O2	000098-00-0	98
2			3-Furanmethanol	98	C5H6O2	004412-91-3	70
3			Methylenecyclopropanecarboxylic ...	98	C5H6O2	062266-36-8	49
4			2,4-Hexadienal, (E,E)-	96	C6H8O	000142-83-6	38
5			Thiocyanic acid, 2-propynyl ester	97	C4H3NS	024309-48-6	27



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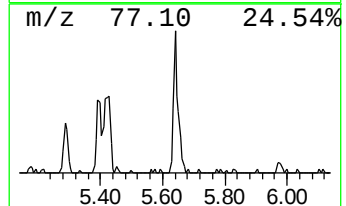
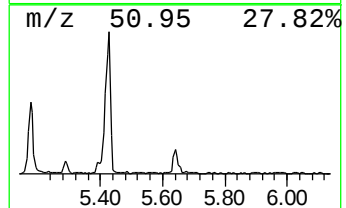
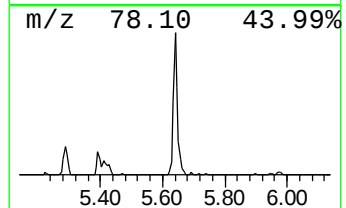
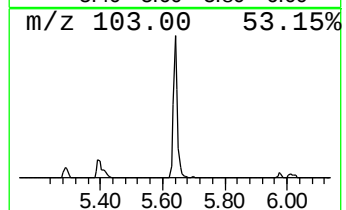
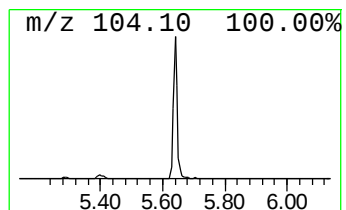
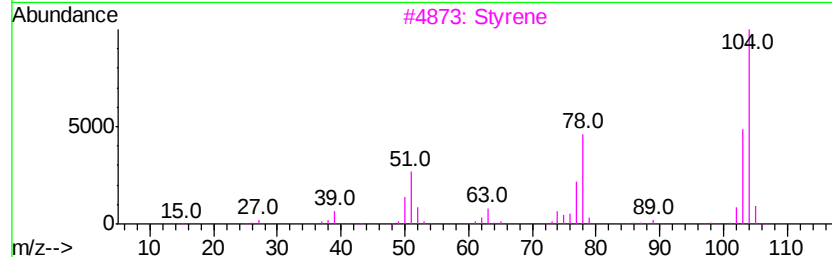
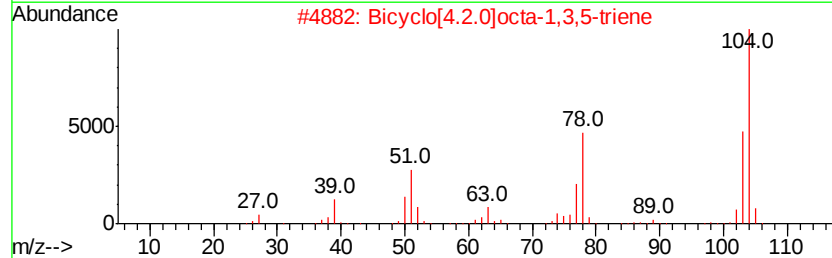
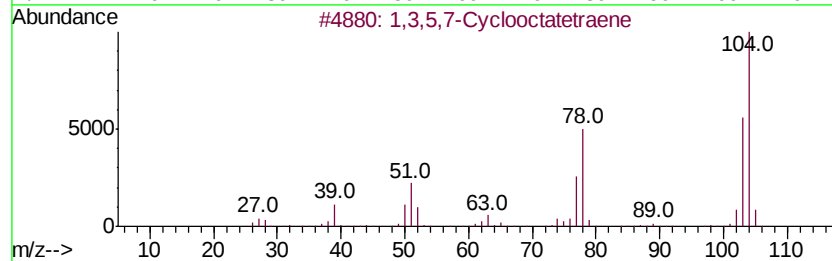
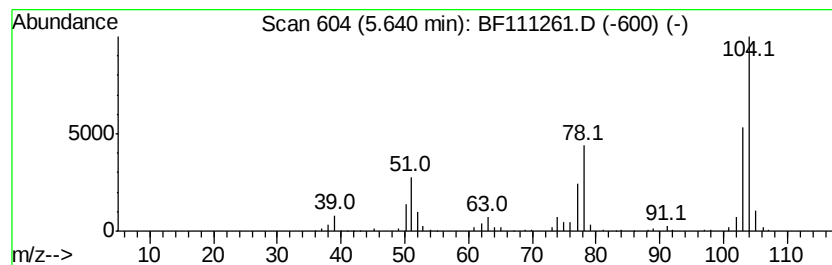
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,3,5,7-Cyclooctatetraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.64	2.35 ng	294538	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	96
2		Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
3		Styrene	104	C8H8	000100-42-5	96
4		Butanedioic acid, phenyl-	194	C10H10O4	000635-51-8	72
5		1,3,7-Octatrien-5-yne	104	C8H8	016607-77-5	28



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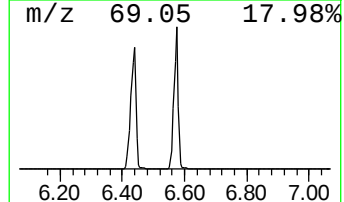
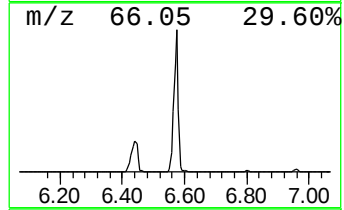
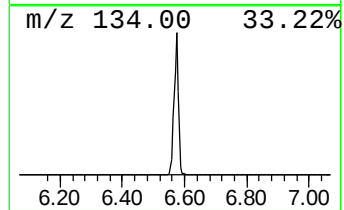
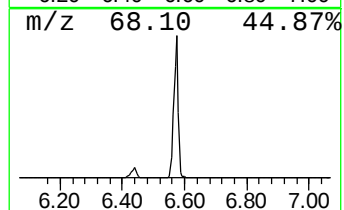
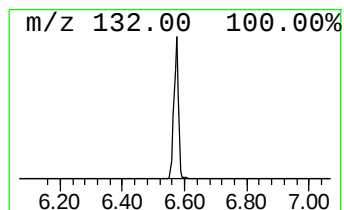
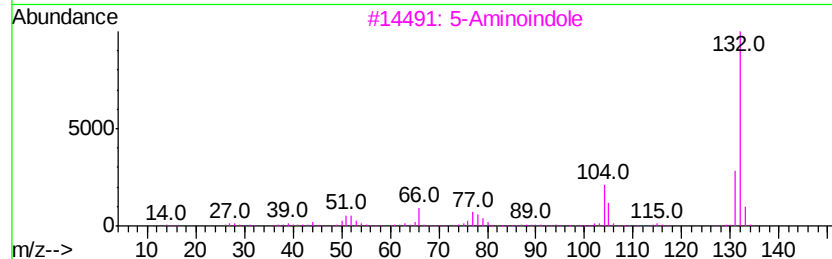
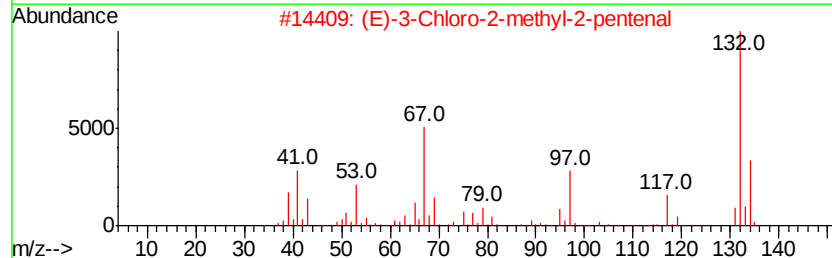
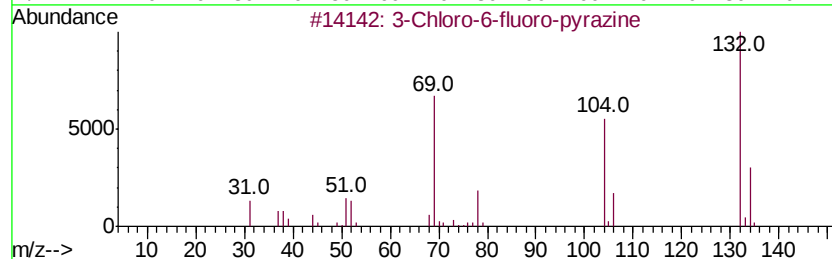
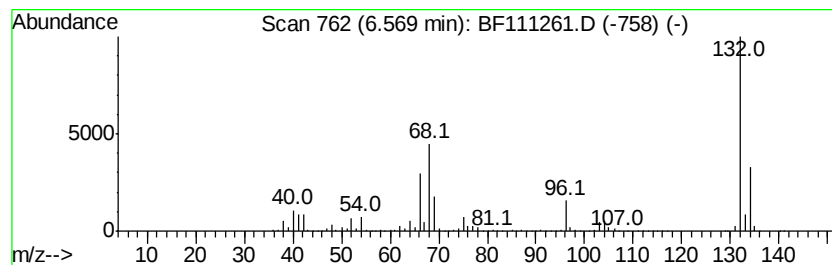
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	94.32 ng	11846800	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12	
3	5-Aminoindole	132	C8H8N2	005192-03-0	12	
4	Amphetaminil	250	C17H18N2	017590-01-1	12	
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9	



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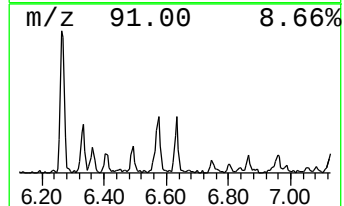
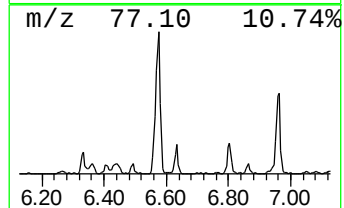
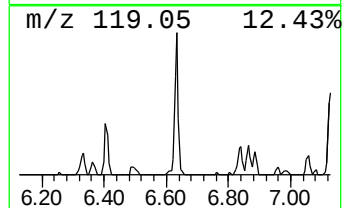
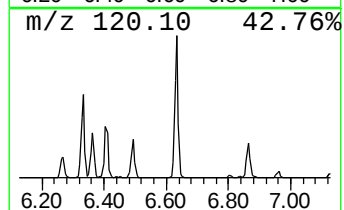
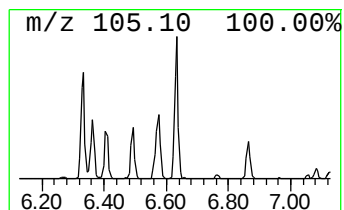
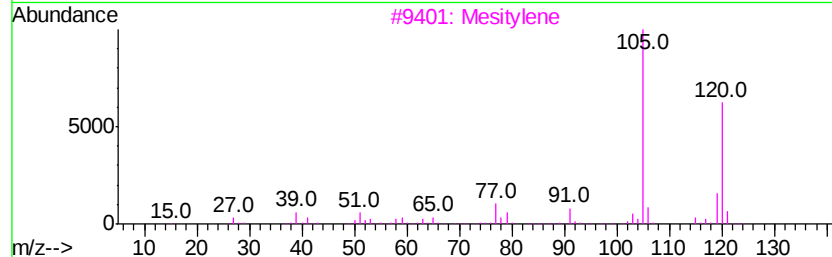
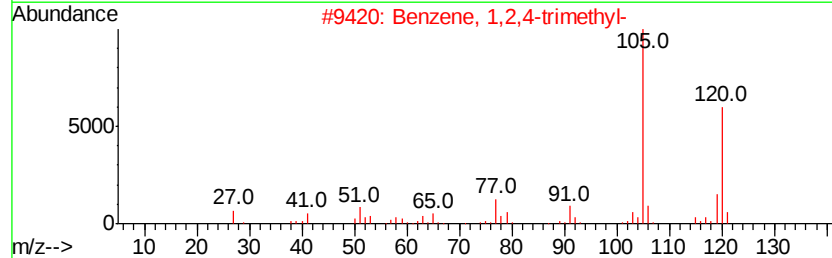
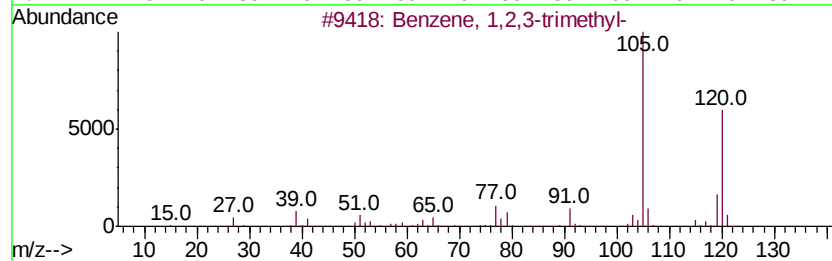
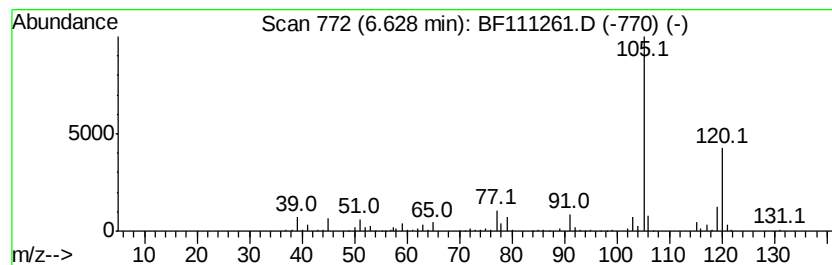
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	2.70 ng	339617	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
3		Mesitylene	120	C9H12	000108-67-8	94
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
Data File : BF111261.D
Acq On : 10 Dec 2018 23:59
Operator : JU/SJ
Sample : J6306-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

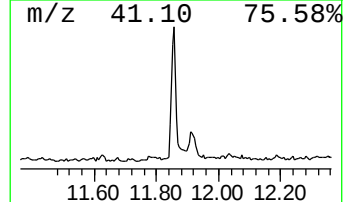
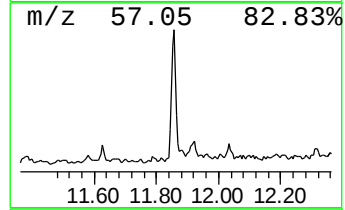
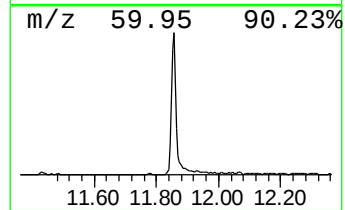
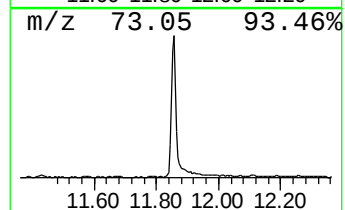
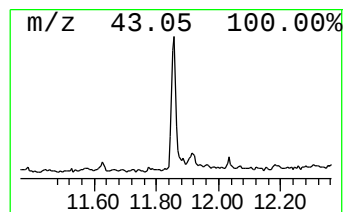
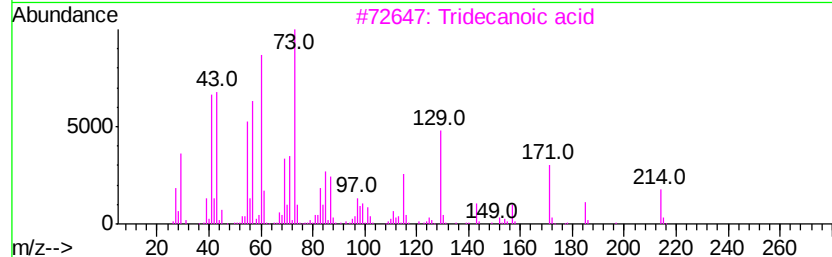
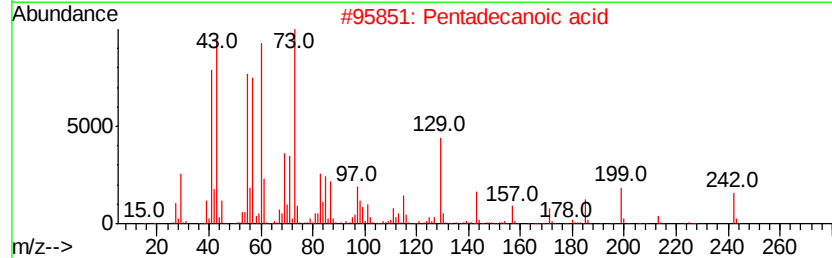
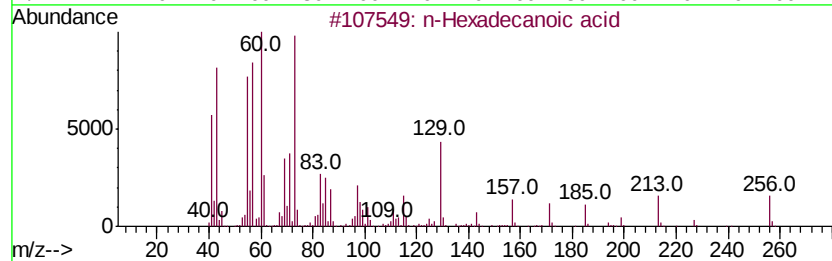
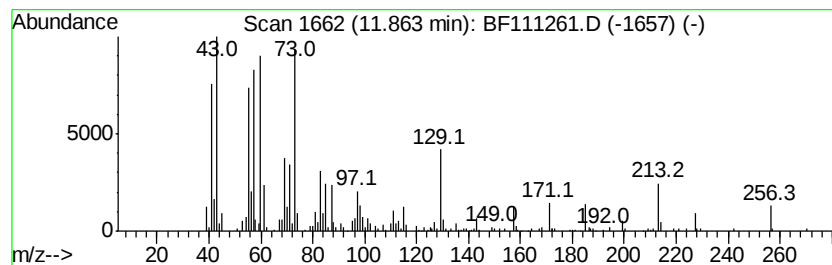
Instrument :
BNA_F
ClientSampleId :
VB-16204

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.86	9.07 ng	978357	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
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Misc :
ALS Vial : 19 Sample Multiplier: 1

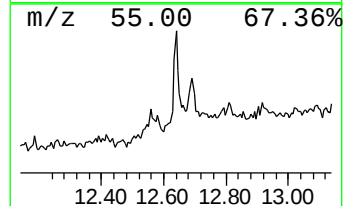
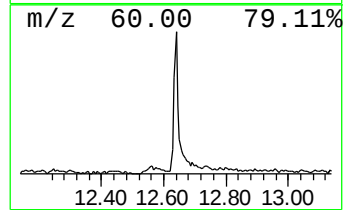
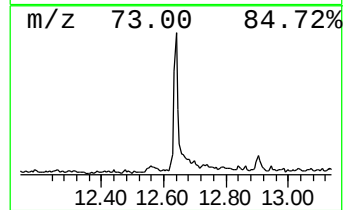
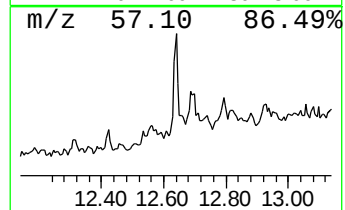
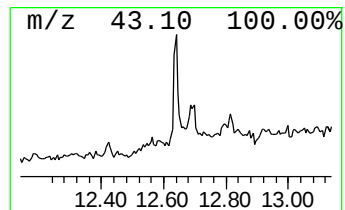
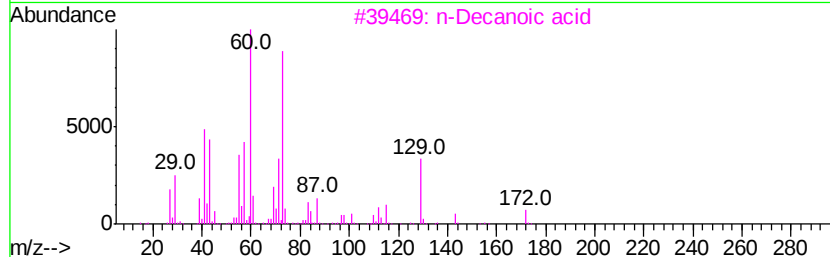
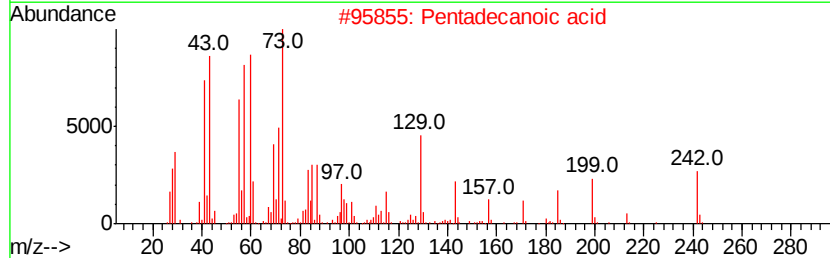
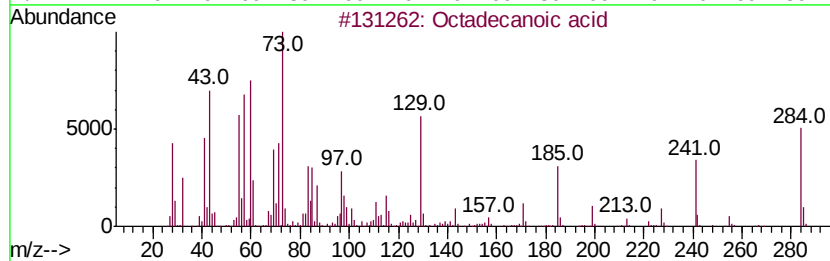
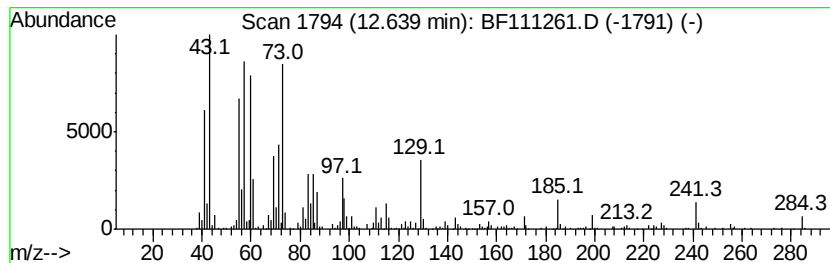
Instrument :
BNA_F
ClientSampleId :
VB-16204

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.64	4.18 ng	451151	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121018\
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Operator : JU/SJ
Sample : J6306-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

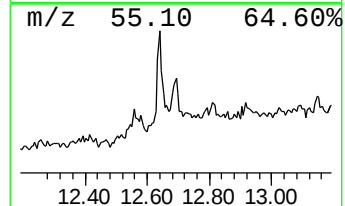
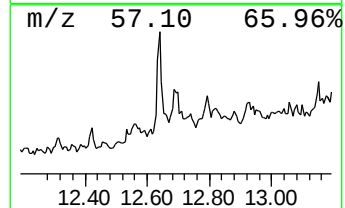
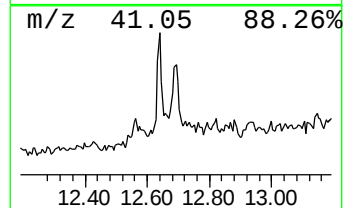
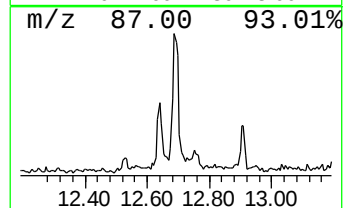
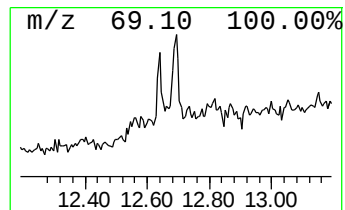
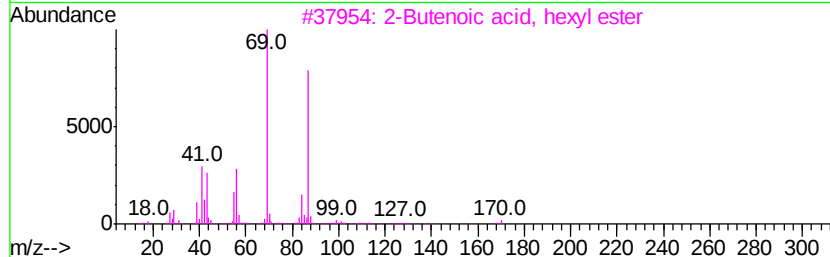
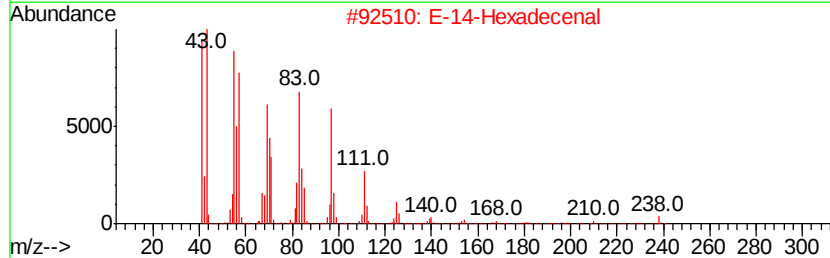
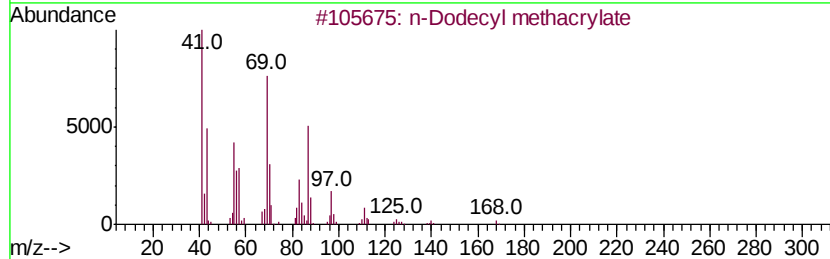
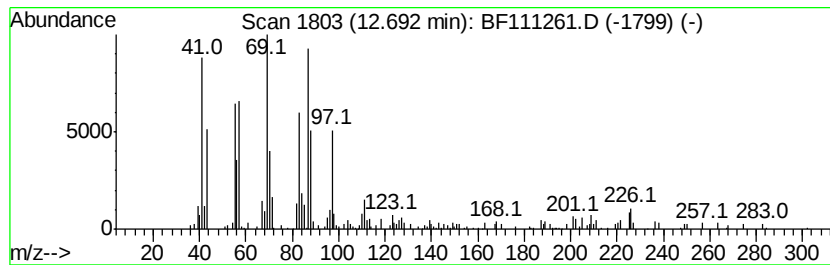
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Dodecyl methacrylate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.69	2.08 ng	233809	Chrysene-d12	13.96	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	64
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	45
3	2-Butenoic acid, hexyl ester	170	C10H18O2	019089-92-0	38
4	3-Trifluoroacetoxy-6-ethyldecane	282	C14H25F3O2	116436-59-0	35
5	1-Dodecene	168	C12H24	000112-41-4	30



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Sample : J6306-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VB-16204

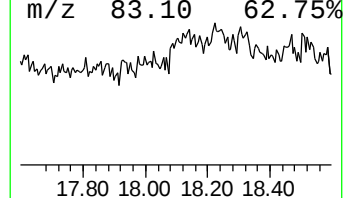
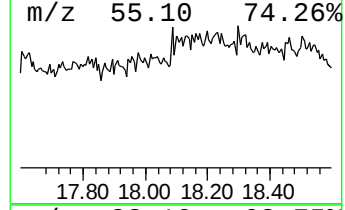
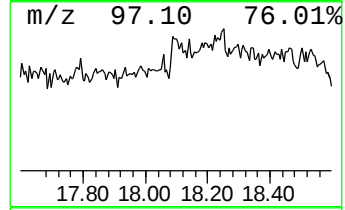
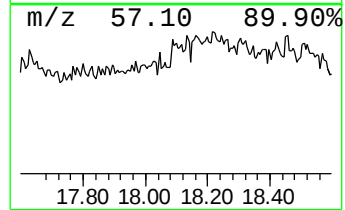
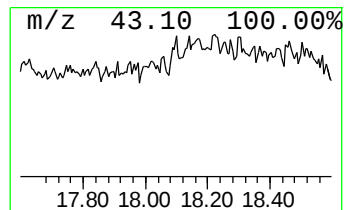
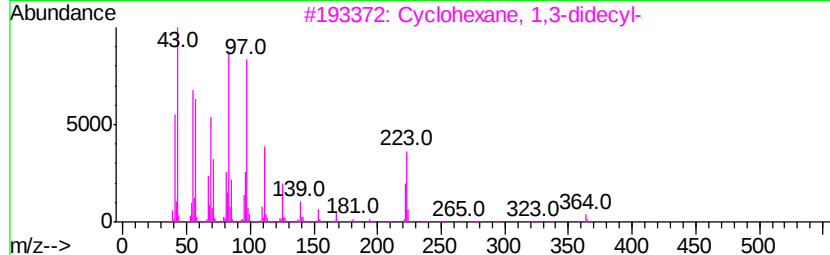
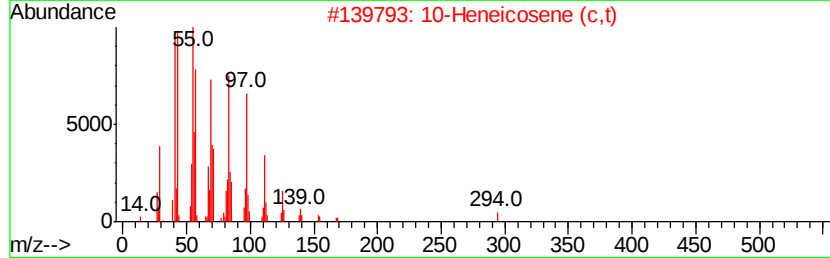
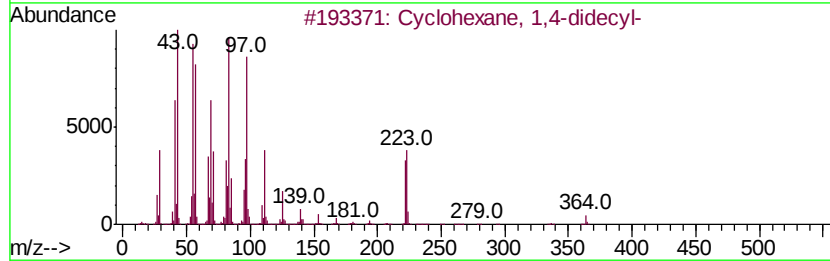
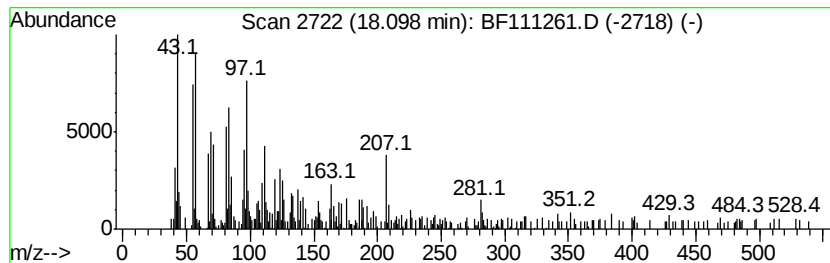
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclohexane, 1,4-didecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.10	2.82 ng	230187	Perylene-d12	15.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,4-didecyl-	364	C26H52	055334-20-8	83
2		10-Heneicosene (c,t)	294	C21H42	095008-11-0	78
3		Cyclohexane, 1,3-didecyl-	364	C26H52	055334-19-5	64
4		1-Docosanethiol	342	C22H46S	007773-83-3	60
5		Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl303	1000314-56-3	50



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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VB-16204

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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...	5.03	5.3	ng	663474	1	6.80	2511970	20.0
2-Furanmethanol	5.17	13.7	ng	1716600	1	6.80	2511970	20.0
1,3,5,7-Cycloocta...	5.64	2.4	ng	294538	1	6.80	2511970	20.0
unknown6.57	6.57	94.3	ng	11846800	1	6.80	2511970	20.0
Benzene, 1,2,3-tr...	6.63	2.7	ng	339617	1	6.80	2511970	20.0
n-Hexadecanoic acid	11.86	9.1	ng	978357	4	11.32	2158300	20.0
Octadecanoic acid	12.64	4.2	ng	451151	4	11.32	2158300	20.0
n-Dodecyl methacr...	12.69	2.1	ng	233809	5	13.96	2246860	20.0
Cyclohexane, 1,4-...	18.10	2.8	ng	230187	6	15.39	1631850	20.0