

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
 Data File : BF109237.D
 Acq On : 22 Sep 2018 22:22
 Operator : JU/SJ
 Sample : J4777-19 2X
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-03-092018-A

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-BF092218.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	4.893	474	477	485	rVB	45808	55648	3.53%	0.346%
2	5.310	544	548	552	rBV	1496835	1355853	86.00%	8.428%
3	6.340	718	723	730	rBV	1622304	1455679	92.33%	9.049%
4	6.475	742	746	749	rBV	1589086	1438277	91.23%	8.940%
5	6.540	754	757	763	rBV	28539	24681	1.57%	0.153%
6	6.704	782	785	789	rBV	874931	704415	44.68%	4.379%
7	6.863	808	812	815	rBV	1428211	1134018	71.93%	7.049%
8	7.263	876	880	883	rBV	1063916	869963	55.18%	5.408%
9	7.986	999	1003	1006	rBV	1111754	875701	55.54%	5.443%
10	9.063	1182	1186	1189	rBV	2059160	1576581	100.00%	9.800%
11	9.192	1204	1208	1211	rBV	412879	379771	24.09%	2.361%
12	9.457	1249	1253	1256	rBV	446171	338798	21.49%	2.106%
13	9.739	1297	1301	1304	rBV	933766	868354	55.08%	5.398%
14	10.328	1397	1401	1406	rBV	47202	51214	3.25%	0.318%
15	10.516	1429	1433	1444	rBV	838914	718071	45.55%	4.464%
16	11.210	1548	1551	1554	rBV	832396	710980	45.10%	4.419%
17	11.233	1554	1555	1558	rVB	65156	35466	2.25%	0.220%
18	11.745	1639	1642	1646	rBV4	18155	24490	1.55%	0.152%
19	12.416	1753	1756	1760	rVB	150243	124482	7.90%	0.774%
20	12.469	1760	1765	1767	rBV2	19659	20420	1.30%	0.127%
21	12.645	1788	1795	1798	rBV	119386	132567	8.41%	0.824%
22	12.792	1816	1820	1823	rBV	1201289	986023	62.54%	6.129%
23	12.974	1844	1851	1854	rBV	19607	32064	2.03%	0.199%
24	13.039	1859	1862	1865	rVB	32929	26615	1.69%	0.165%
25	13.074	1865	1868	1872	rBV	19532	19921	1.26%	0.124%
26	13.380	1917	1920	1922	rBV	27372	22506	1.43%	0.140%
27	13.586	1951	1955	1958	rBV2	17523	23837	1.51%	0.148%
28	13.710	1973	1976	1982	rBV3	30201	43665	2.77%	0.271%
29	13.833	1993	1997	2000	rBV	742001	763592	48.43%	4.747%
30	13.863	2000	2002	2006	rVB	68453	61339	3.89%	0.381%
31	14.021	2026	2029	2032	rBV2	35808	32110	2.04%	0.200%
32	14.327	2077	2081	2083	rBV	43035	52112	3.31%	0.324%
33	14.621	2128	2131	2134	rVB	44625	43095	2.73%	0.268%
34	14.751	2151	2153	2157	rVB3	54209	54115	3.43%	0.336%

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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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35	14.839	2165	2168	2176	rBV	63911	121202	7.69%	0.753%
36	14.933	2181	2184	2189	rVB2	85315	98033	6.22%	0.609%
37	15.174	2222	2225	2231	rVB	47341	52136	3.31%	0.324%
38	15.233	2231	2235	2240	rBV	435510	509798	32.34%	3.169%
39	15.286	2242	2244	2249	rVB	57143	58806	3.73%	0.366%
40	15.686	2309	2312	2317	rVB	79746	109880	6.97%	0.683%
41	16.151	2387	2391	2400	rVB3	41510	81066	5.14%	0.504%

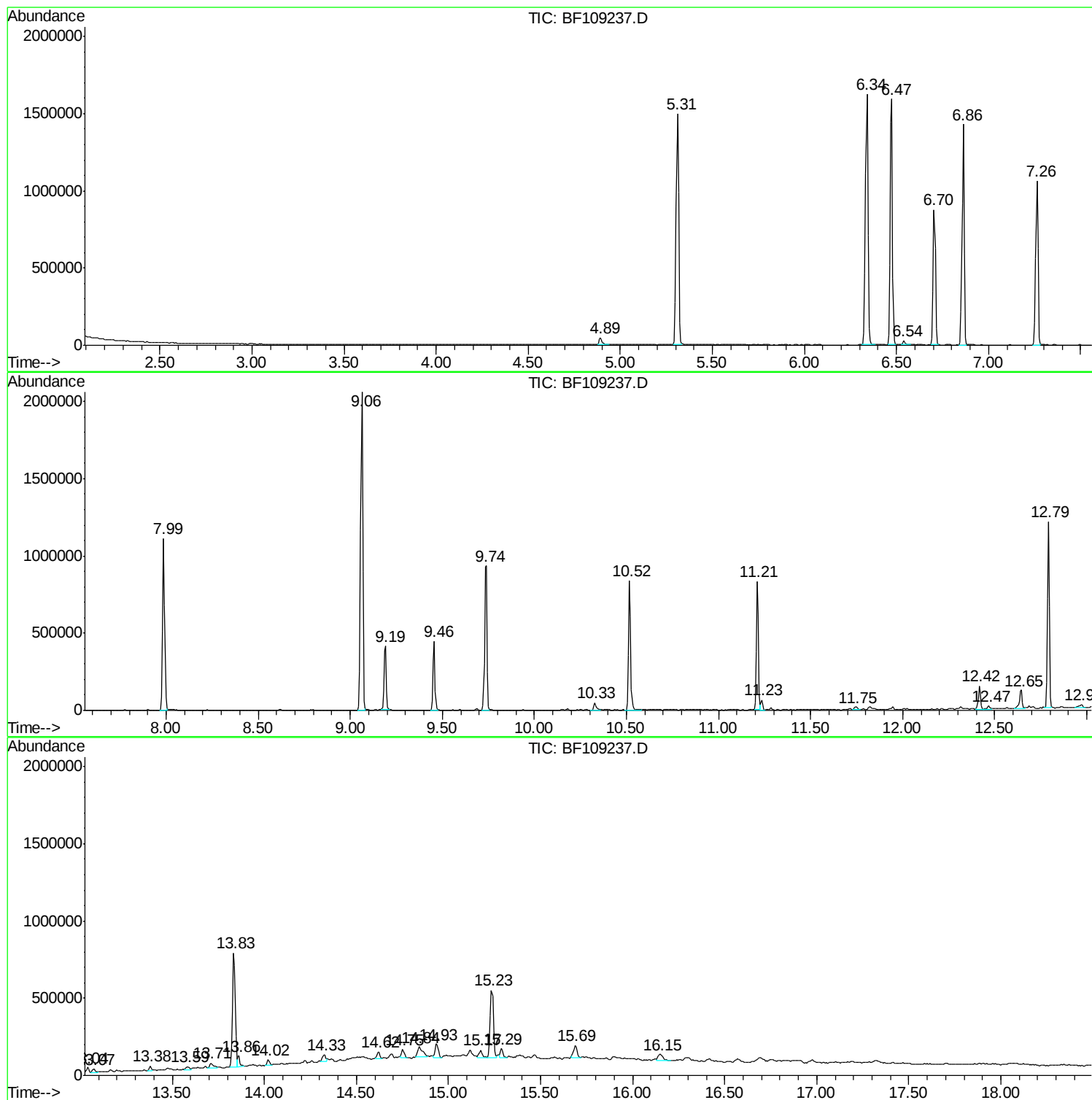
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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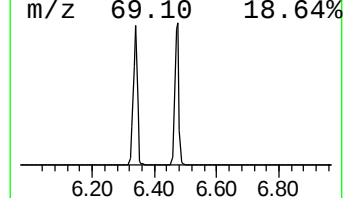
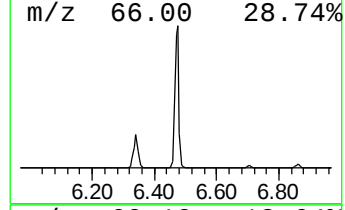
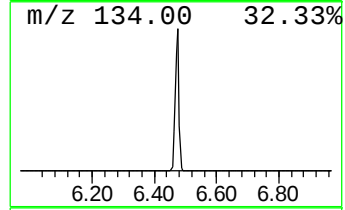
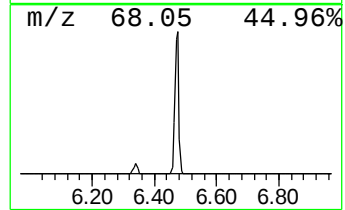
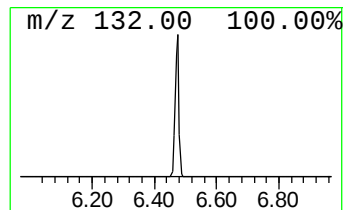
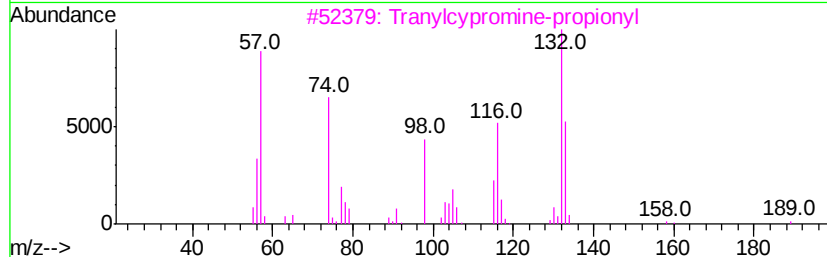
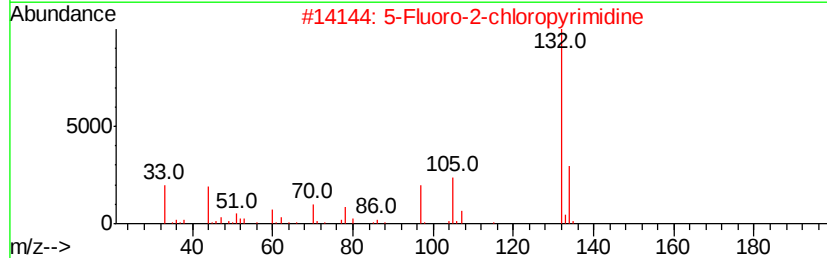
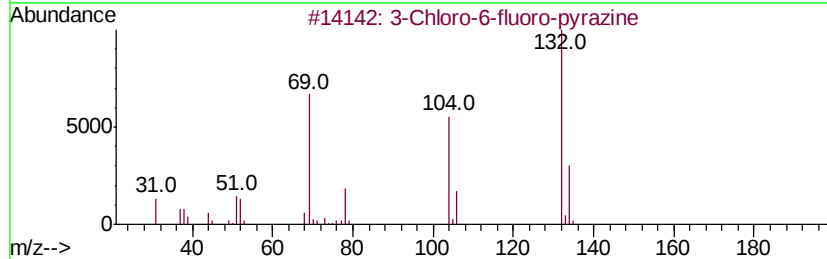
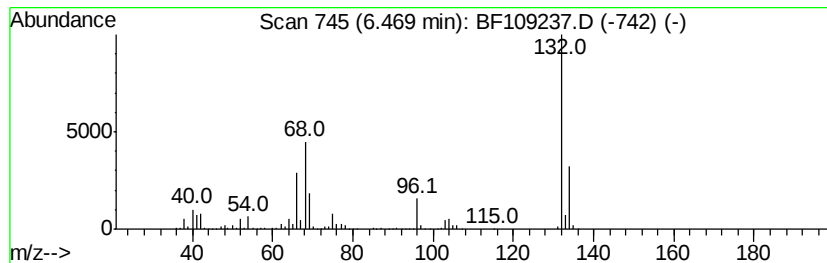
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	40.84 ng	1438280	1,4-Dichlorobenzene-d4	6.70

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		Tranvlcypramine-propionyl	189	C12H15NO	1000123-86-3	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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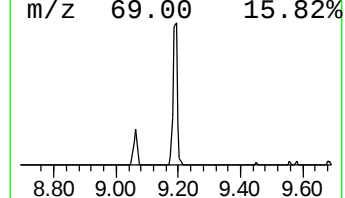
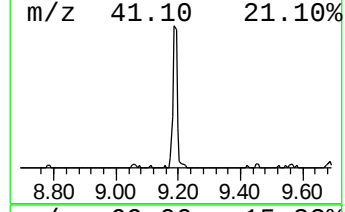
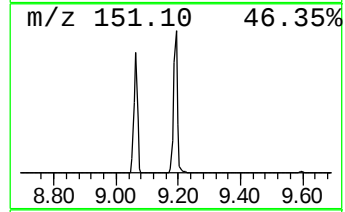
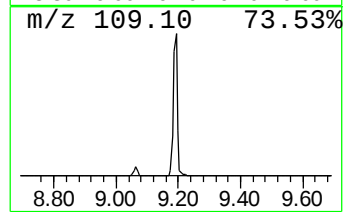
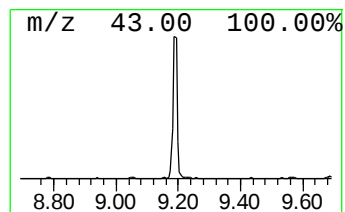
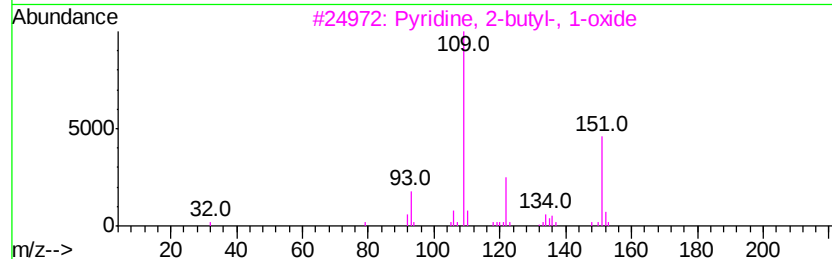
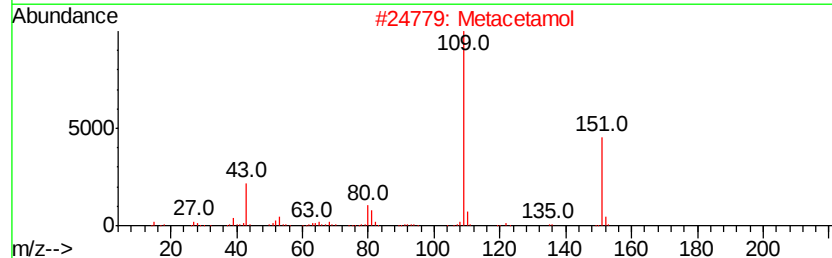
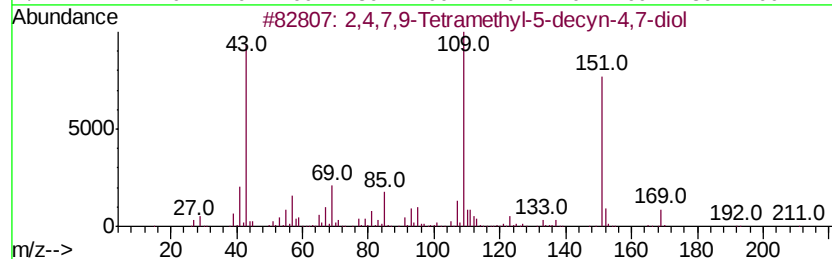
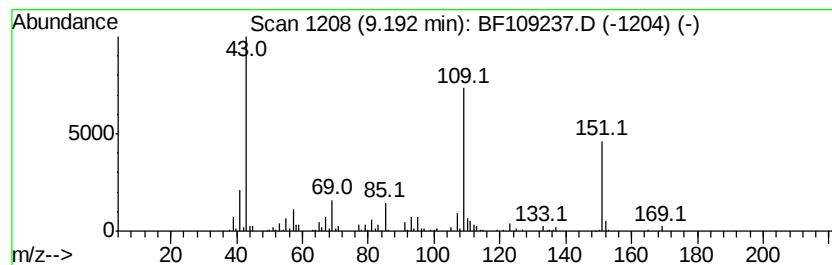
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
9.19	8.75 ng	379771	Acenaphthene-d10	9.73	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	64
3	Pvridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	59
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59
5	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	59



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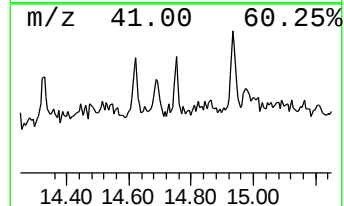
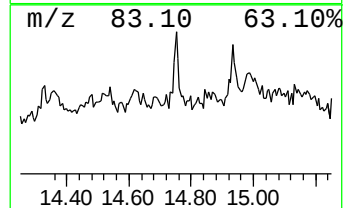
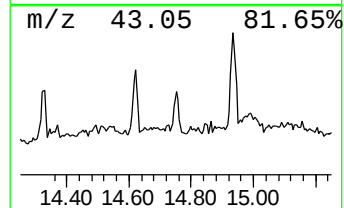
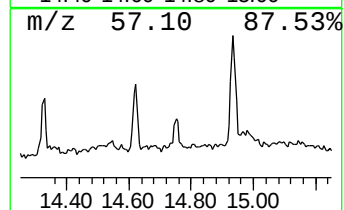
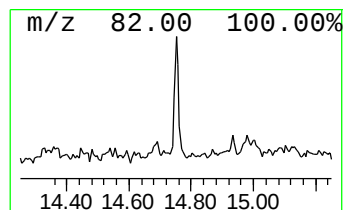
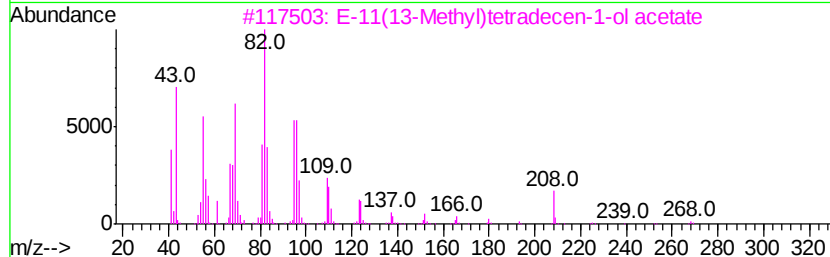
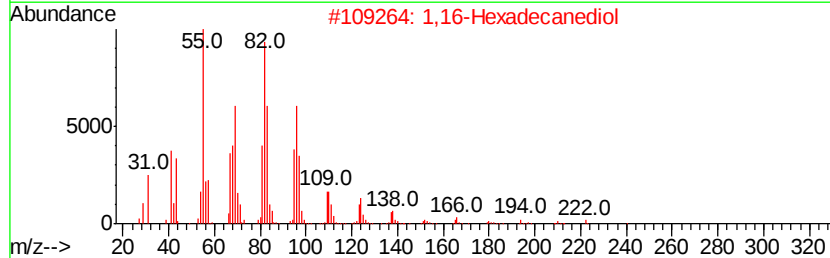
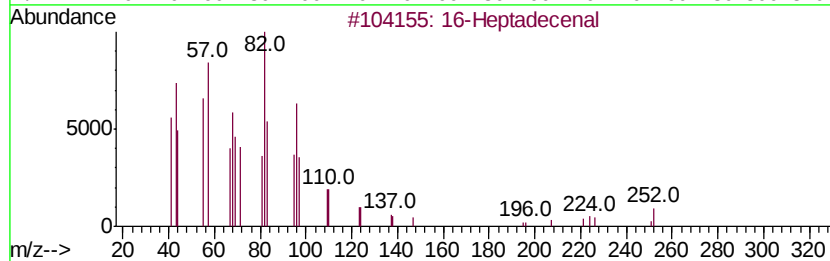
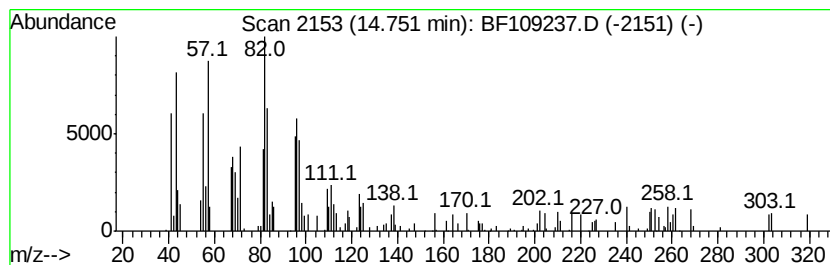
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 16-Heptadecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.12 ng	54115	Perylene-d12	15.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Heptadecenal	252	C17H32O	1000144-57-9	83
2		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	64
3		E-11(13-Methyl)tetradecen-1-ol a...	268	C17H32O2	1000130-80-4	58
4		10-Methyl-E-11-tridecen-1-ol pro...	268	C17H32O2	1000130-97-4	50
5		Oxacyclohexadecan-2-one	240	C15H28O2	000106-02-5	50



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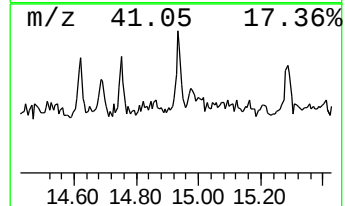
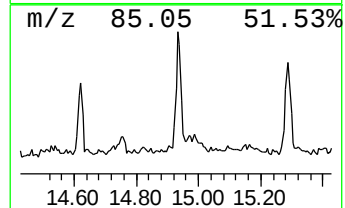
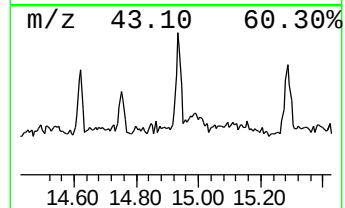
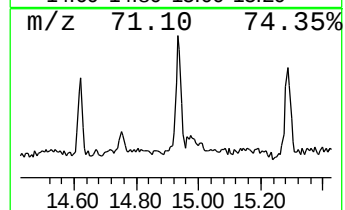
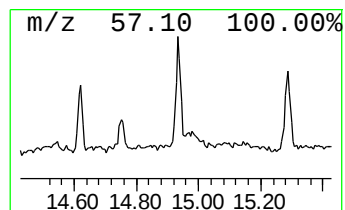
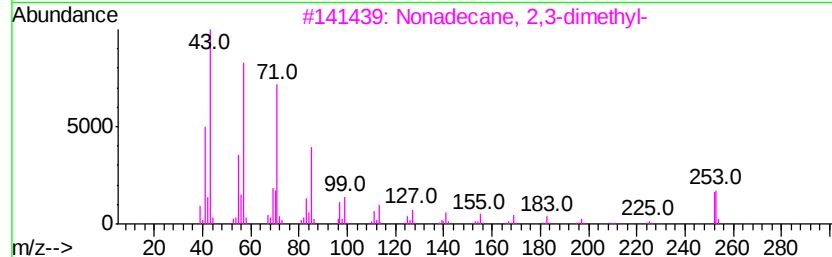
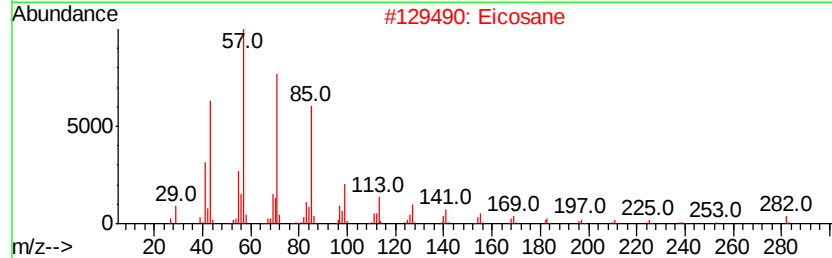
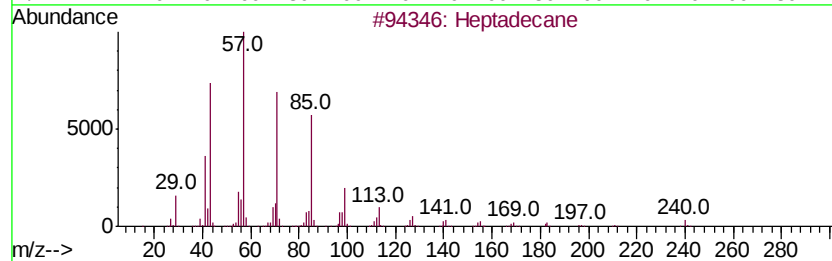
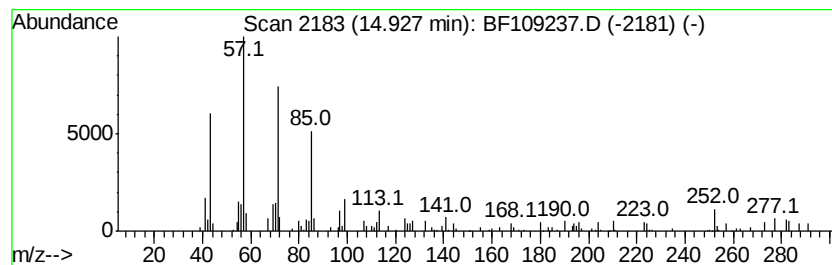
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.93	3.85 ng	98033	Perylene-d12		15.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	96
2	Eicosane	282	C20H42	000112-95-8	95
3	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexacosane	366	C26H54	000630-01-3	83



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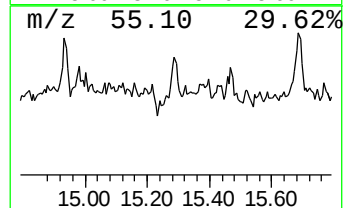
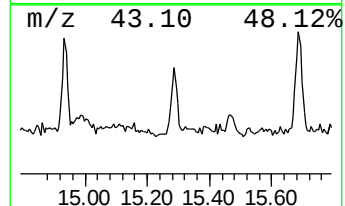
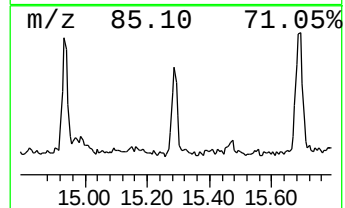
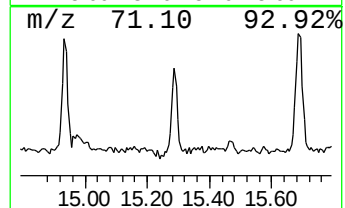
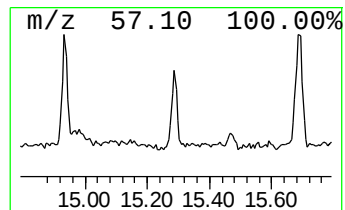
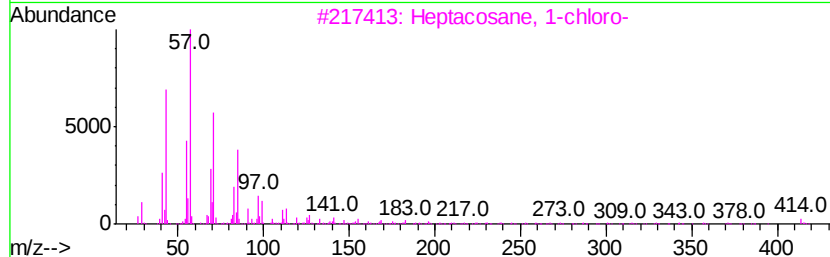
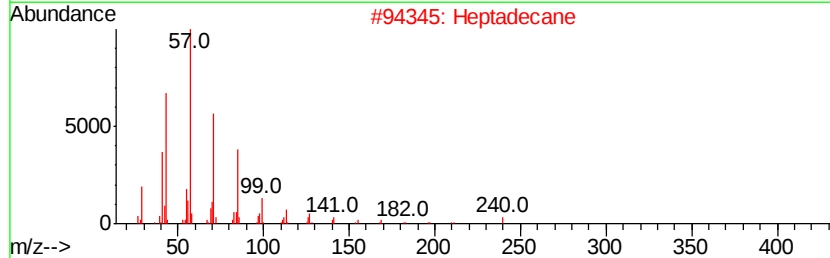
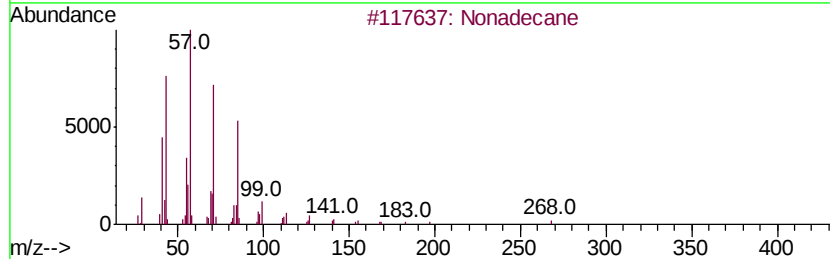
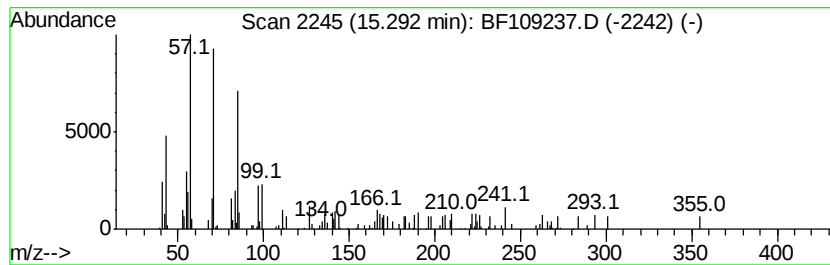
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
15.29	2.31 ng	58806	Perylene-d12		15.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	74
2	Heptadecane	240	C17H36	000629-78-7	72
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
4	Tetratetracontane	619	C44H90	007098-22-8	72
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109237.D
Acq On : 22 Sep 2018 22:22
Operator : JU/SJ
Sample : J4777-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-A

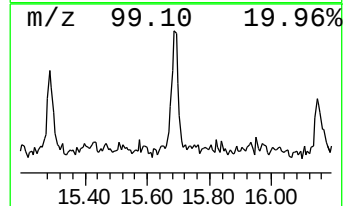
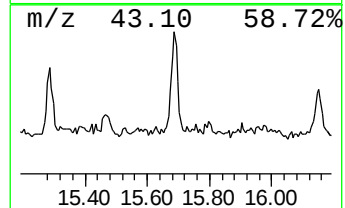
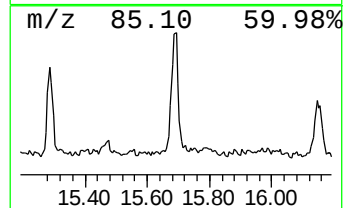
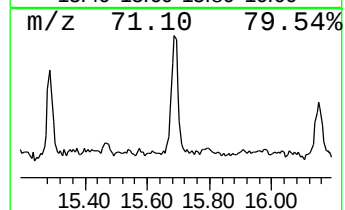
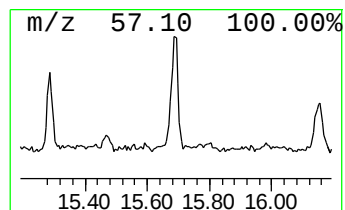
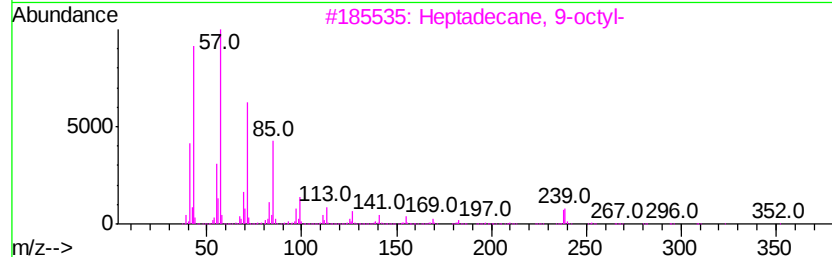
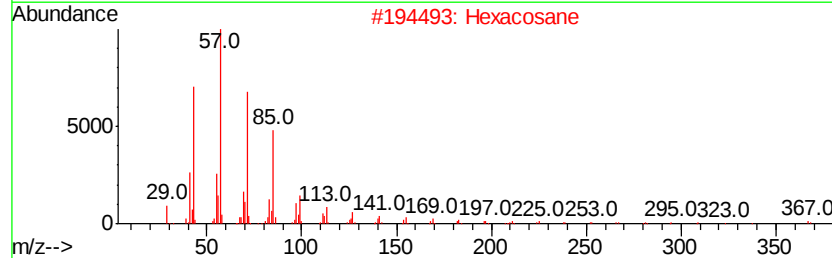
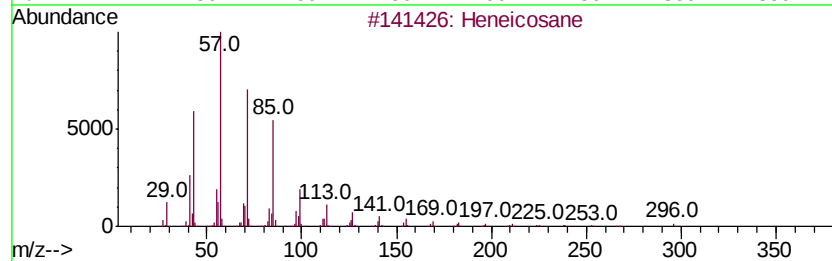
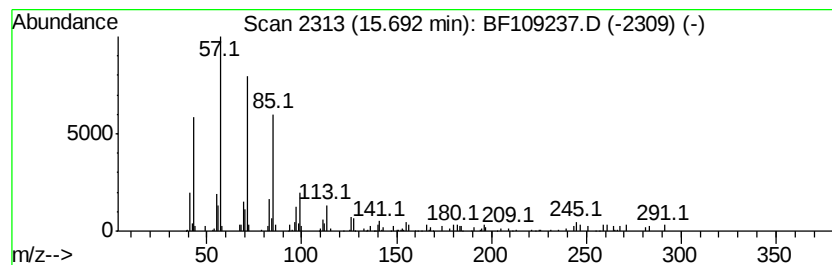
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	4.31 ng	109880	Perylene-d12	15.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Hexacosane		366	C26H54	000630-01-3	87
3	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	87
4	Tetracosane		338	C24H50	000646-31-1	87
5	Docosane, 7-hexyl-		394	C28H58	055373-86-9	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
Data File : BF109237.D
Acq On : 22 Sep 2018 22:22
Operator : JU/SJ
Sample : J4777-19 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
unknown6.47	6.47	40.8	ng	1438280	1	6.70	704415	20.0
2,4,7,9-Tetrameth...	9.19	8.8	ng	379771	3	9.73	868354	20.0
16-Heptadecenal	14.75	2.1	ng	54115	6	15.23	509798	20.0
Heptadecane	14.93	3.9	ng	98033	6	15.23	509798	20.0
Nonadecane	15.29	2.3	ng	58806	6	15.23	509798	20.0
Heneicosane	15.69	4.3	ng	109880	6	15.23	509798	20.0