

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
 Data File : BF117588.D
 Acq On : 29 Oct 2019 14:04
 Operator : JU
 Sample : K5503-15
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 172-22-(0-2)

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-BF101819.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	4.934	480	484	495	rBV	17320	29090	3.16%	0.383%
2	5.357	553	556	584	rBV	613554	792592	86.04%	10.445%
3	6.386	727	731	748	rBV	730062	895777	97.24%	11.805%
4	6.504	748	751	764	rVB	971340	921199	100.00%	12.140%
5	6.728	786	789	797	rBV	249676	226011	24.53%	2.979%
6	6.881	812	815	830	rBV	650994	598099	64.93%	7.882%
7	7.292	882	885	908	rBV	425778	522007	56.67%	6.879%
8	8.010	1004	1007	1029	rBV	236424	274463	29.79%	3.617%
9	9.080	1186	1189	1206	rBV	790251	716545	77.78%	9.443%
10	9.480	1254	1257	1267	rBV	63536	67011	7.27%	0.883%
11	9.763	1301	1305	1318	rBV	248645	264983	28.77%	3.492%
12	10.557	1436	1440	1450	rBV	294244	339665	36.87%	4.476%
13	11.251	1554	1558	1560	rBV	192831	187950	20.40%	2.477%
14	11.268	1560	1561	1568	rVB	44814	45266	4.91%	0.597%
15	11.774	1645	1647	1654	rVB3	20106	25723	2.79%	0.339%
16	11.868	1659	1663	1665	rBV	9311	10117	1.10%	0.133%
17	12.463	1761	1764	1770	rBV	74295	72703	7.89%	0.958%
18	12.568	1779	1782	1789	rBV3	4747	10154	1.10%	0.134%
19	12.692	1797	1803	1810	rBV	71509	80422	8.73%	1.060%
20	12.827	1822	1826	1830	rBV	539892	450874	48.94%	5.942%
21	13.398	1919	1923	1925	rBV	12210	13838	1.50%	0.182%
22	13.727	1976	1979	1990	rVB4	49704	97392	10.57%	1.284%
23	13.892	2002	2007	2010	rBV2	238640	257136	27.91%	3.389%
24	13.921	2010	2012	2019	rVB	38222	41137	4.47%	0.542%
25	14.039	2029	2032	2034	rBV	22890	21044	2.28%	0.277%
26	14.286	2069	2074	2077	rBV3	9236	15019	1.63%	0.198%
27	14.345	2081	2084	2087	rVV	33646	31062	3.37%	0.409%
28	14.404	2090	2094	2098	rVB	56193	67655	7.34%	0.892%
29	14.639	2131	2134	2140	rVB2	47214	46551	5.05%	0.613%
30	14.709	2143	2146	2149	rVB	38407	34432	3.74%	0.454%
31	14.921	2179	2182	2185	rBV	34067	47219	5.13%	0.622%
32	14.956	2185	2188	2191	rVB3	46701	55755	6.05%	0.735%
33	15.215	2229	2232	2236	rVB2	16319	16960	1.84%	0.224%
34	15.274	2239	2242	2245	rBV	25252	28057	3.05%	0.370%

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35	15.327	2245	2251	2261	rVB	139248	221654	24.06%	2.921%
36	15.715	2312	2317	2320	rVB	26311	35950	3.90%	0.474%
37	15.945	2354	2356	2360	rVB4	8643	9626	1.04%	0.127%
38	16.180	2394	2396	2400	rVB3	13972	16753	1.82%	0.221%

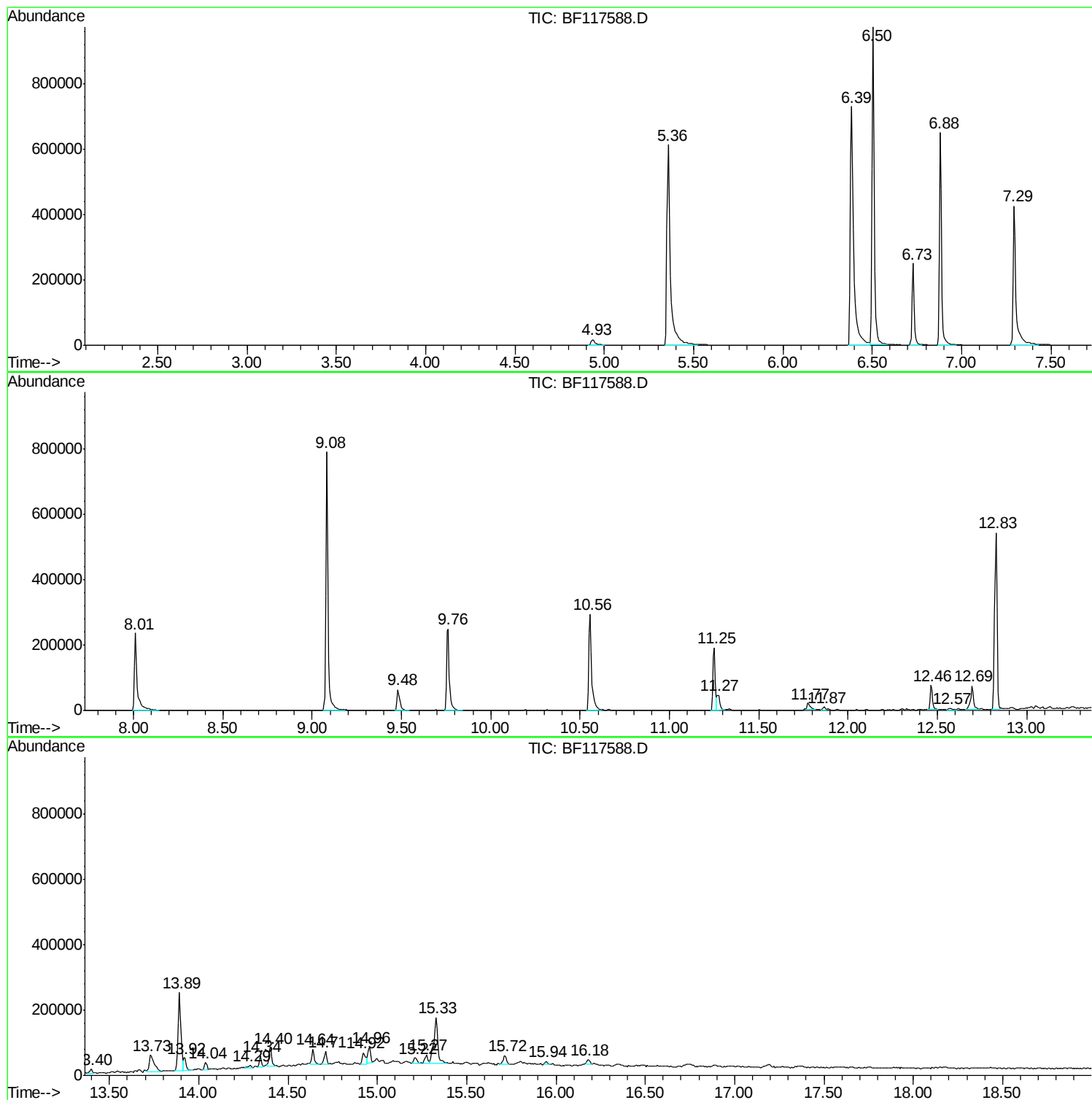
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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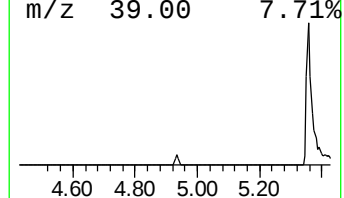
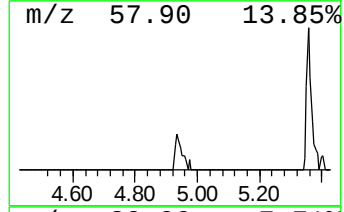
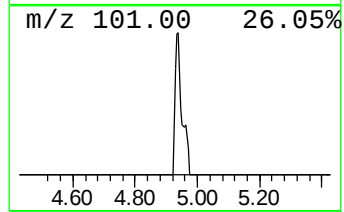
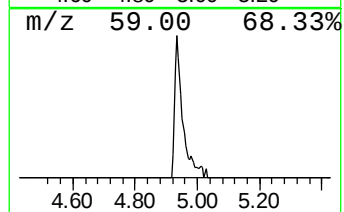
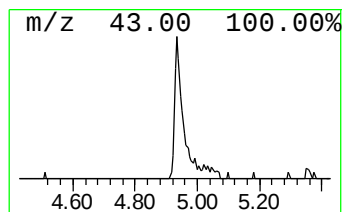
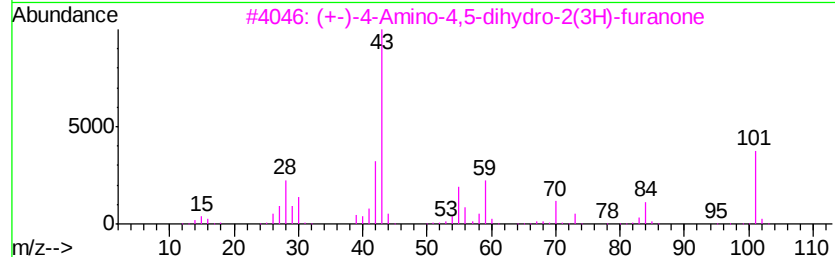
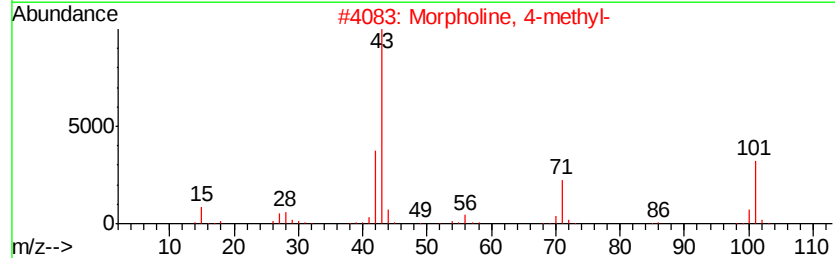
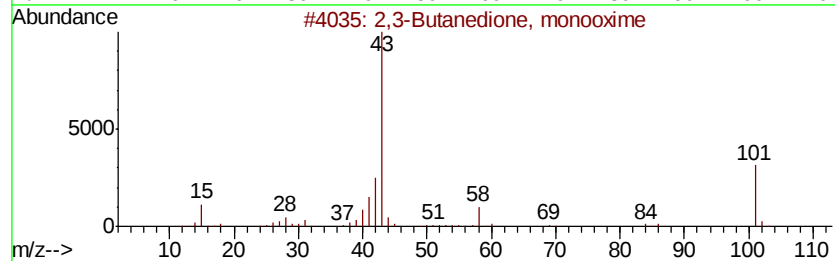
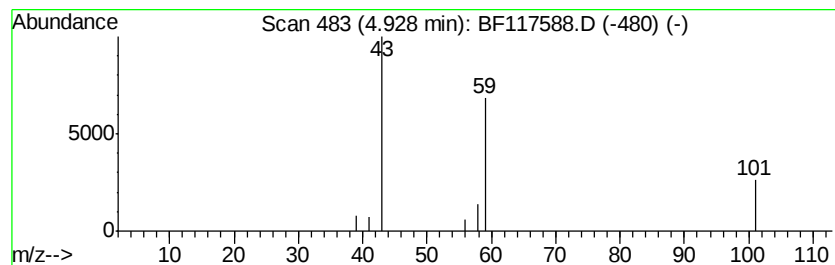
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown4.93 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.57 ng	29090	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	5
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
3			(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	5
4			Diacetamide	101	C4H7NO2	000625-77-4	4
5			Guanidine	59	CH5N3	000113-00-8	4



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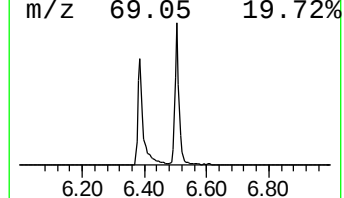
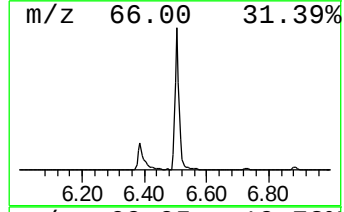
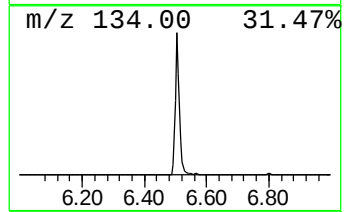
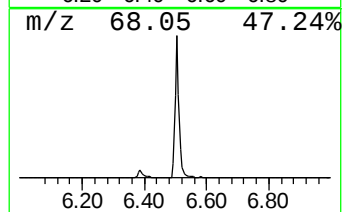
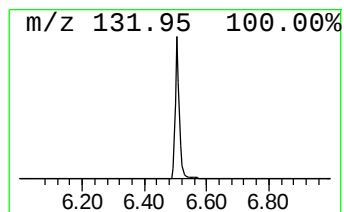
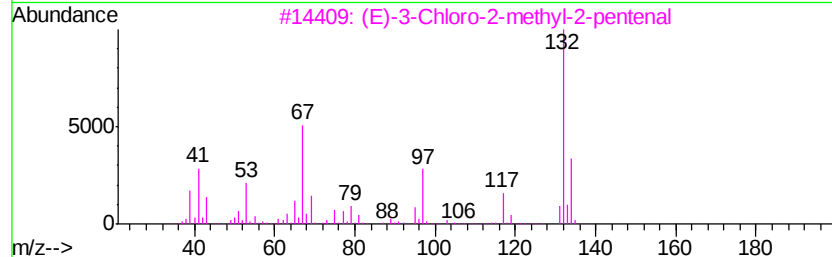
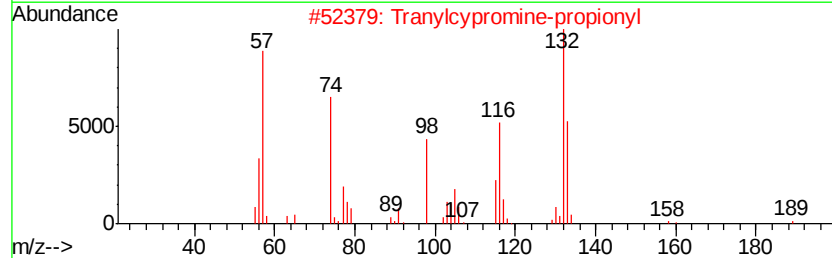
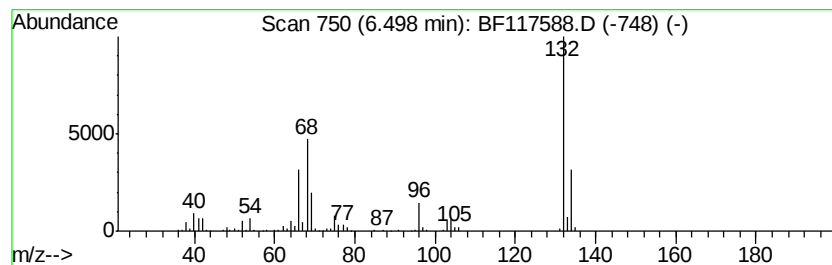
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	81.52 ng	921199	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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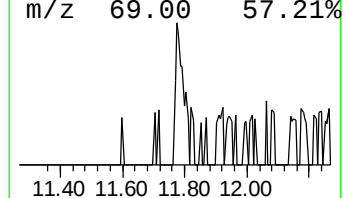
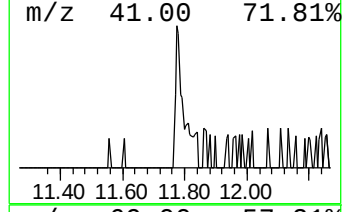
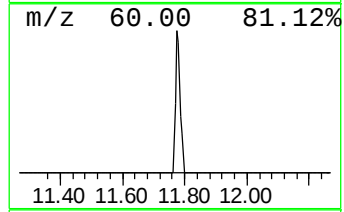
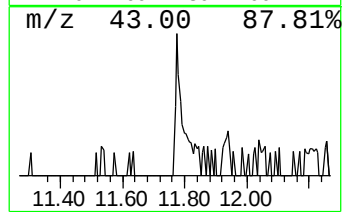
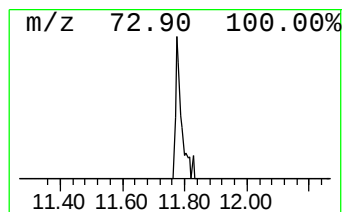
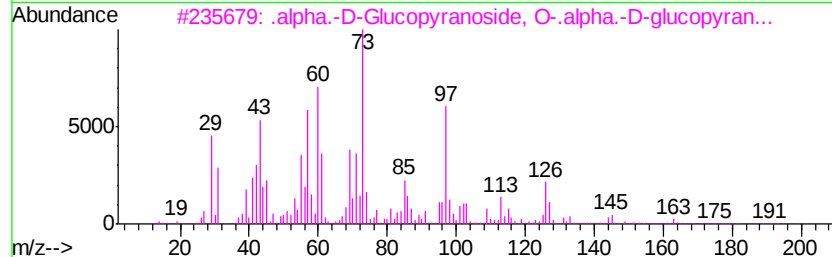
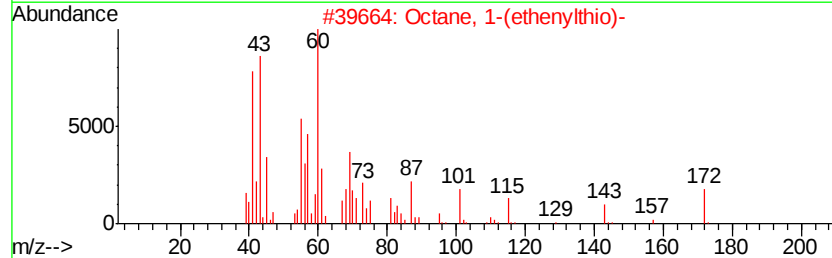
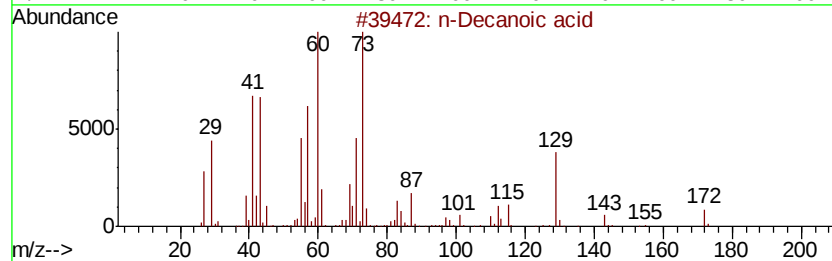
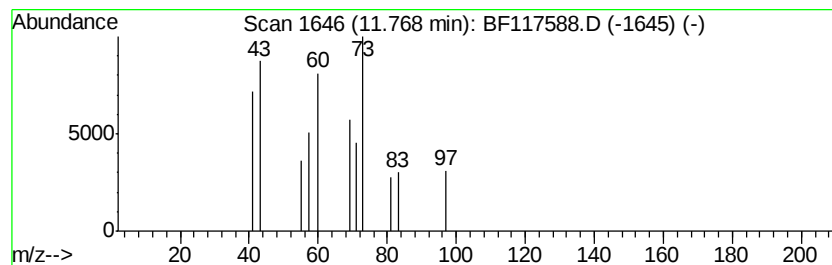
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown11.77 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.74 ng	25723	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	38
2		Octane, 1-(ethenylthio)-	172	C10H20S	042779-08-8	35
3		.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	32
4		.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	27
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	25



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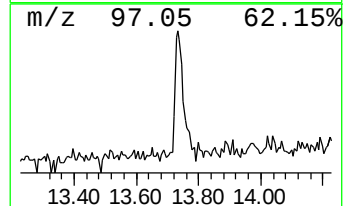
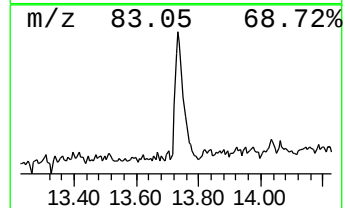
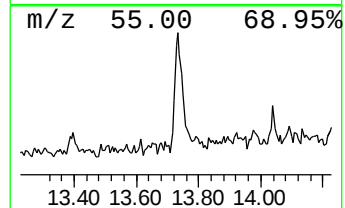
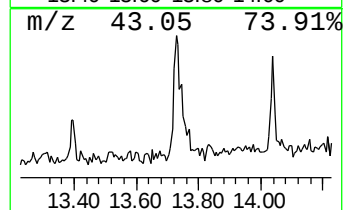
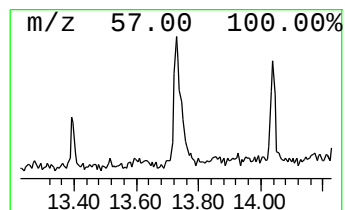
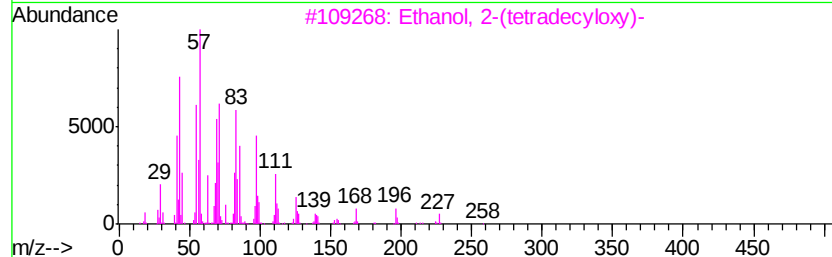
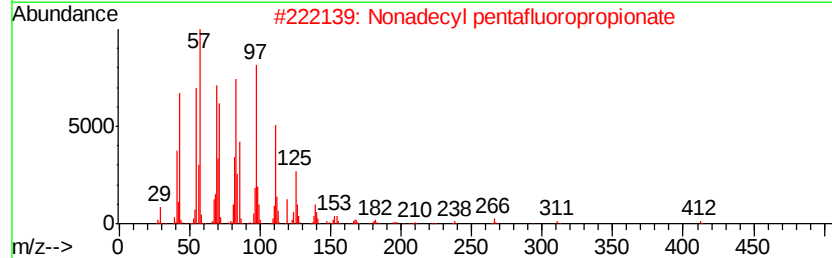
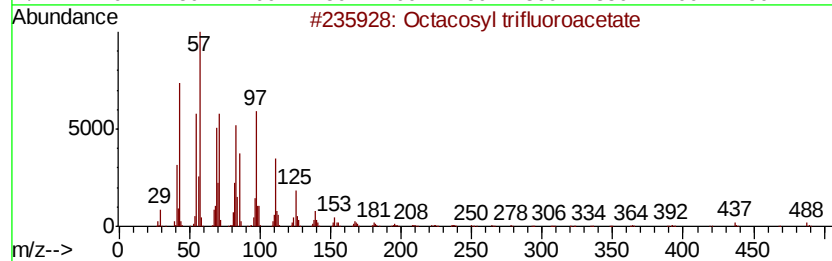
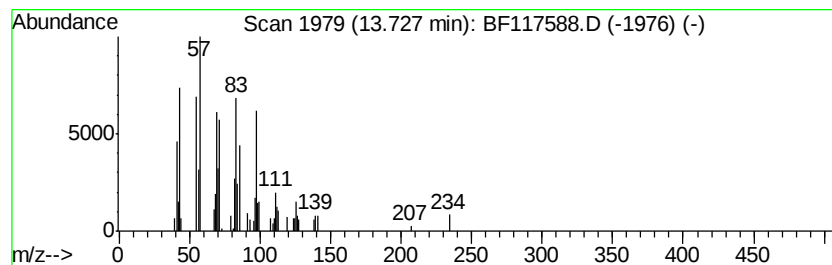
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.58 ng	97392	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
3		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
4		Heneicosyl heptafluorobutyrat	508	C25H43F7O2	1000351-83-8	83
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	76



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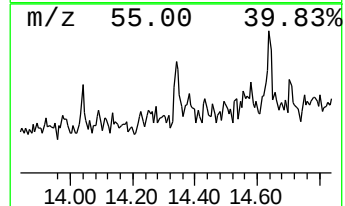
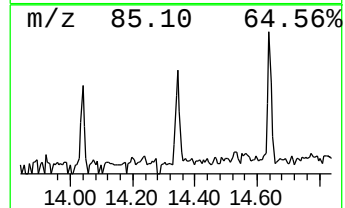
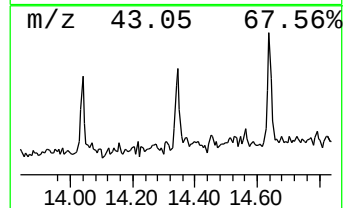
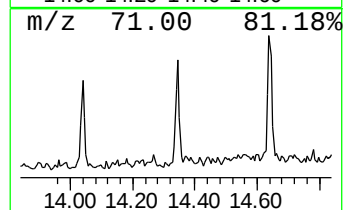
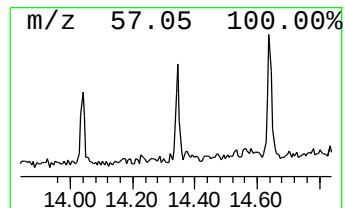
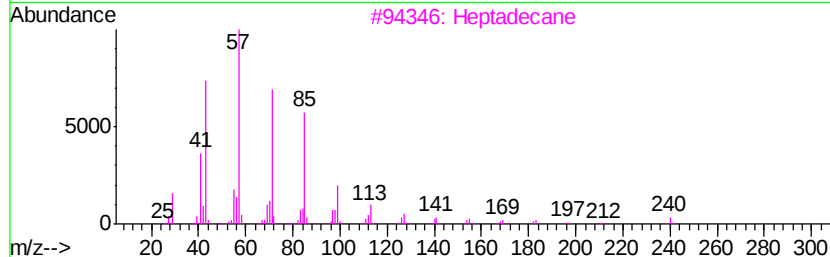
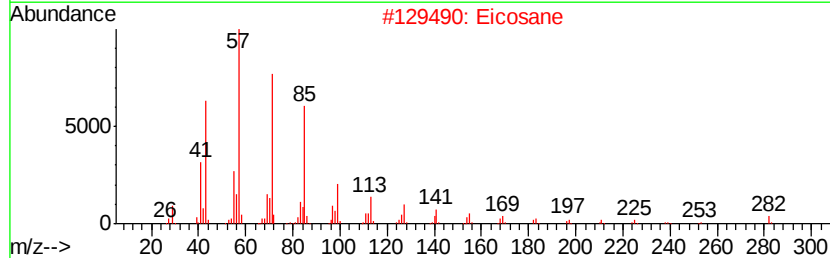
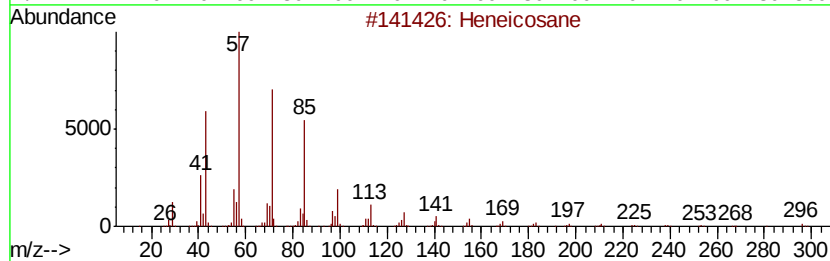
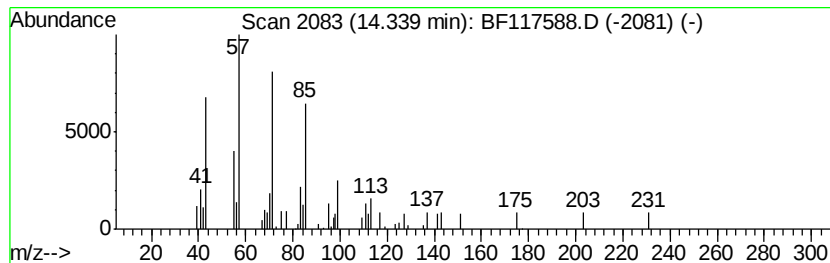
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Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.42 ng	31062	Chrysene-d12	13.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	90
2	Eicosane		282	C20H42	000112-95-8	87
3	Heptadecane		240	C17H36	000629-78-7	87
4	Octacosane		394	C28H58	000630-02-4	87
5	triacontane		422	C30H62	000638-68-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117588.D
Acq On : 29 Oct 2019 14:04
Operator : JU
Sample : K5503-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
172-22-(0-2)

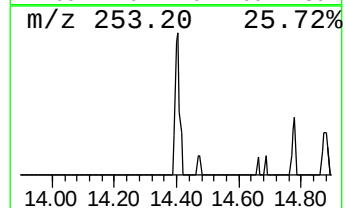
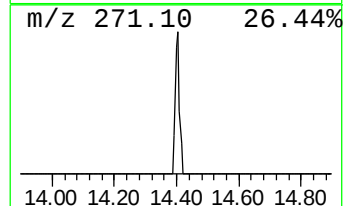
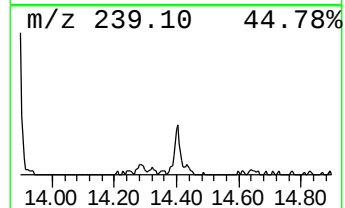
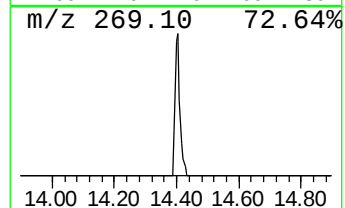
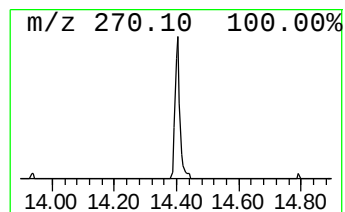
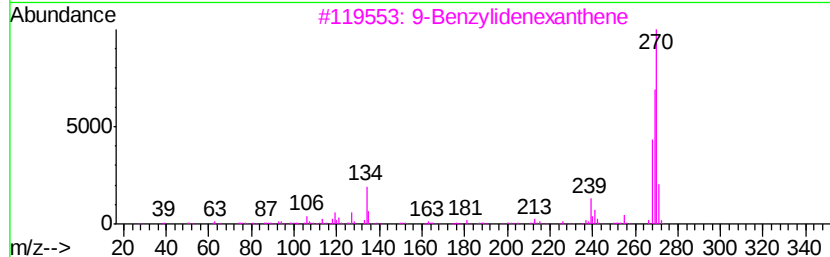
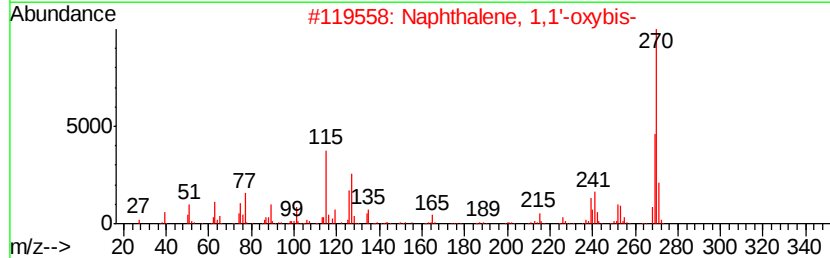
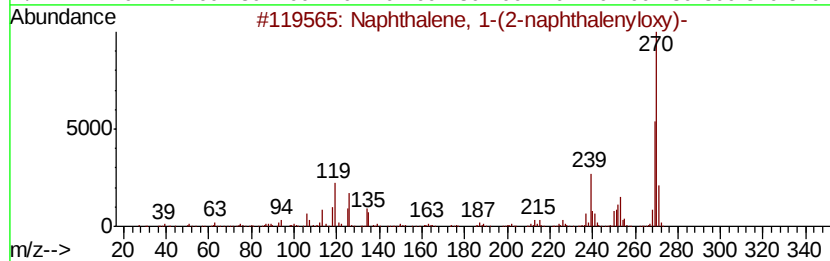
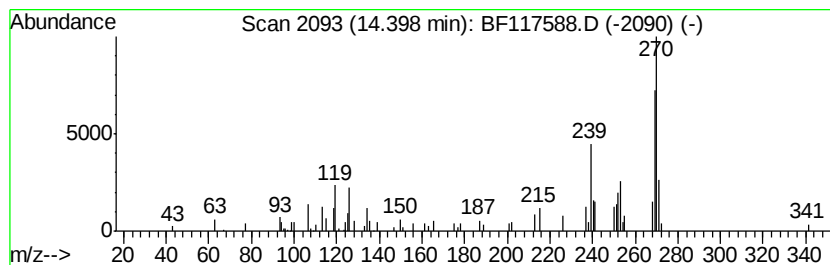
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Naphthalene, 1-(2-naphthale... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	5.26 ng	67655	Chrysene-d12	13.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-(2-naphthalenyloxy)-	270	C20H14O	000611-49-4	95
2		Naphthalene, 1,1'-oxybis-	270	C20H14O	000607-52-3	76
3		9-Benzylidenexanthene	270	C20H14O	027980-52-5	64
4		4-Azafluorenone, 3-methylphenyli...	270	C19H14N2	1000301-74-7	49
5		Benz(a)anthracene, 7,10,12-trime...	270	C21H18	035187-27-0	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117588.D
Acq On : 29 Oct 2019 14:04
Operator : JU
Sample : K5503-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
172-22-(0-2)

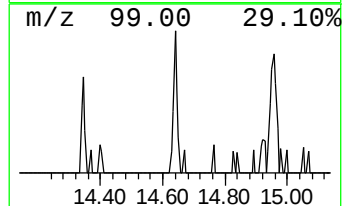
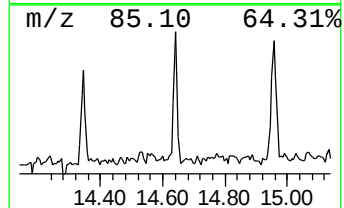
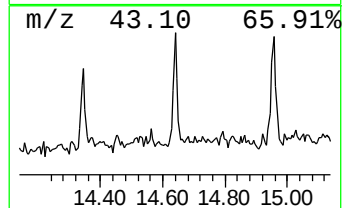
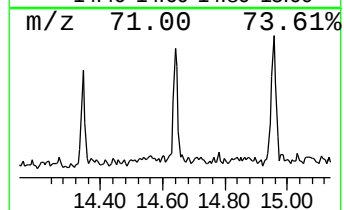
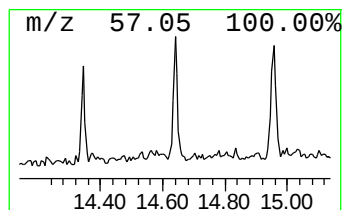
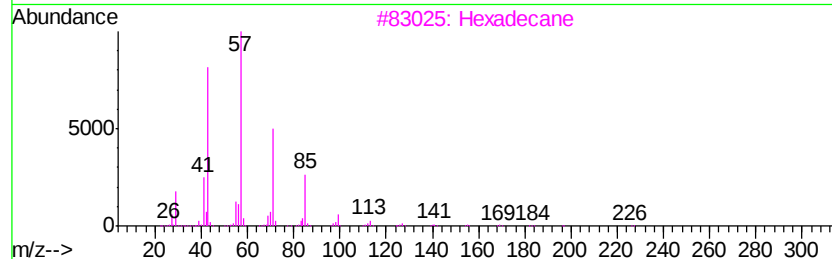
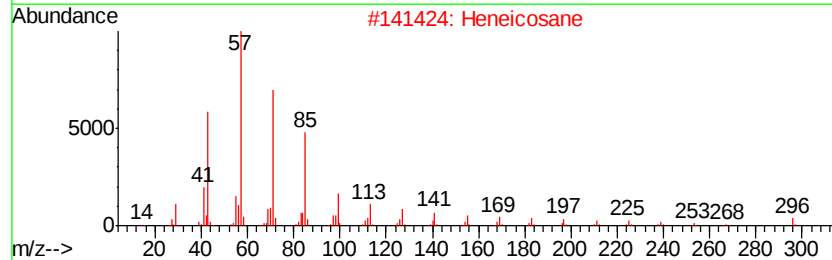
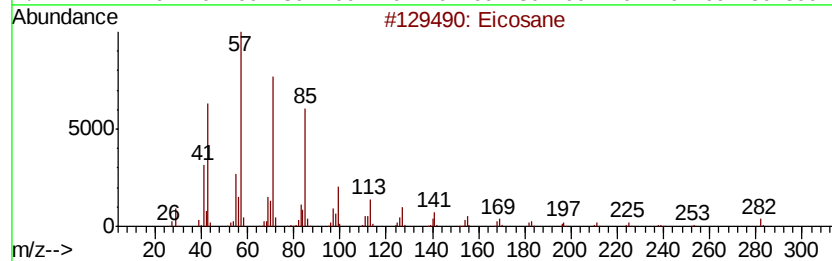
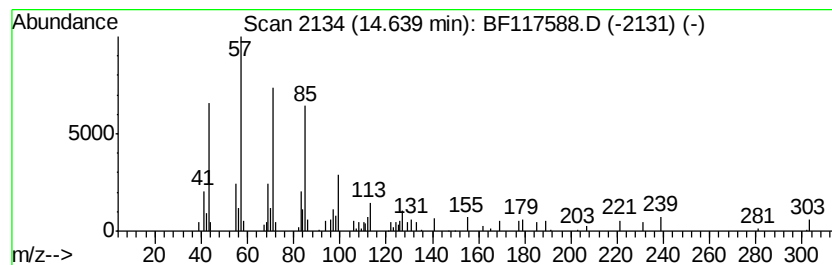
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.20 ng	46551	Perylene-d12	15.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	83
2	Heneicosane		296	C21H44	000629-94-7	83
3	Hexadecane		226	C16H34	000544-76-3	80
4	Heptadecane		240	C17H36	000629-78-7	80
5	6,6-Diethylhoctadecane		310	C22H46	1000360-41-8	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117588.D
Acq On : 29 Oct 2019 14:04
Operator : JU
Sample : K5503-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
172-22-(0-2)

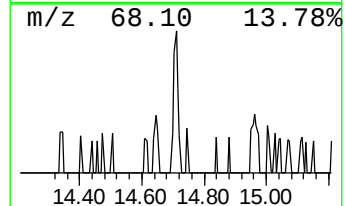
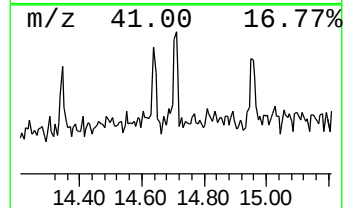
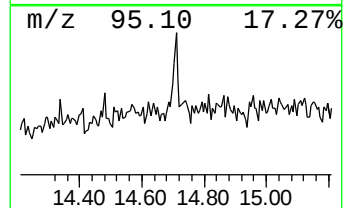
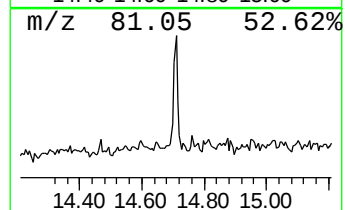
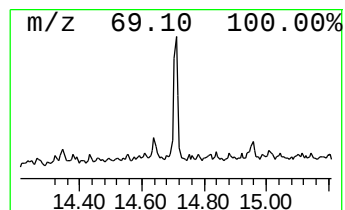
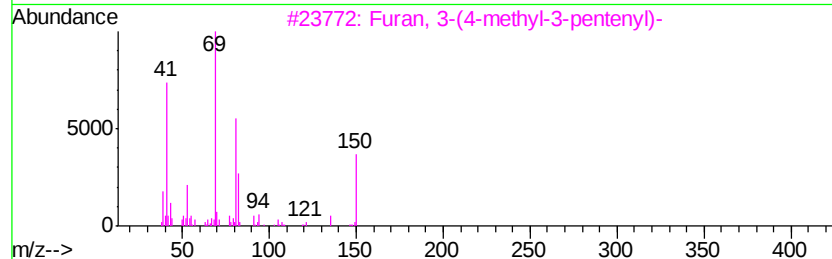
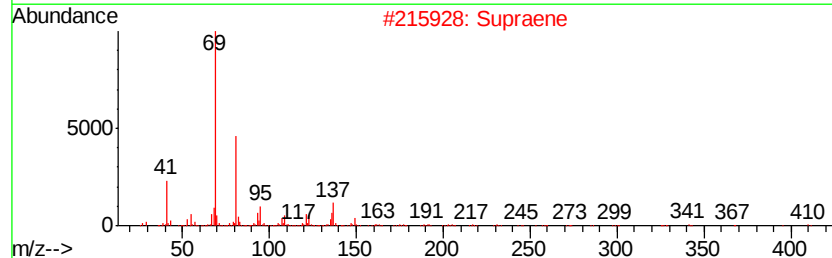
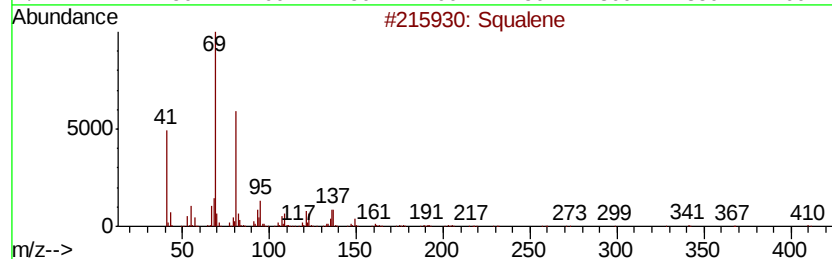
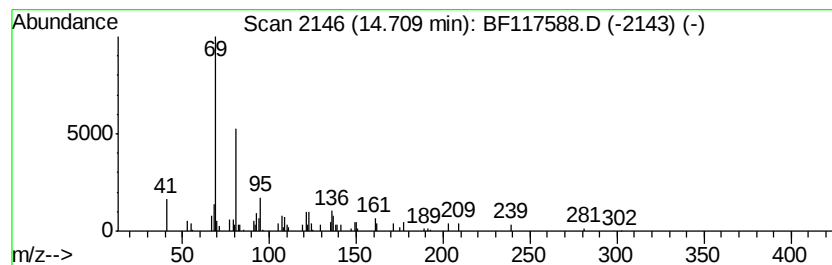
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	3.11 ng	34432	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Supraene	410	C30H50	007683-64-9	80
3		Furan, 3-(4-methyl-3-pentenyl)-	150	C10H14O	000539-52-6	43
4		2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	43
5		Pentane, 1,5-dibromo-	228	C5H10Br2	000111-24-0	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102919\
Data File : BF117588.D
Acq On : 29 Oct 2019 14:04
Operator : JU
Sample : K5503-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
172-22-(0-2)

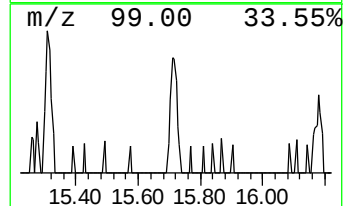
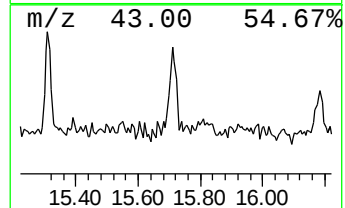
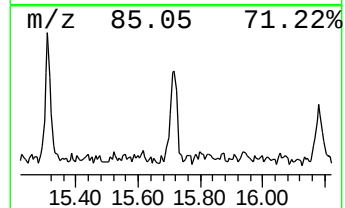
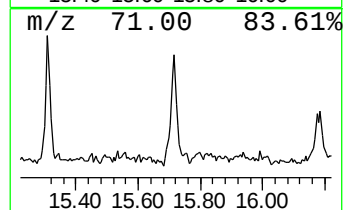
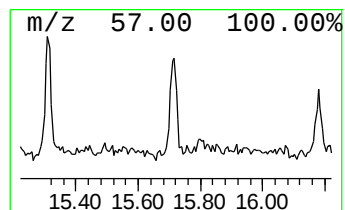
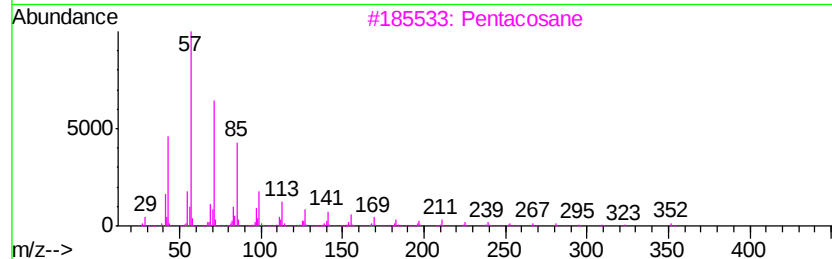
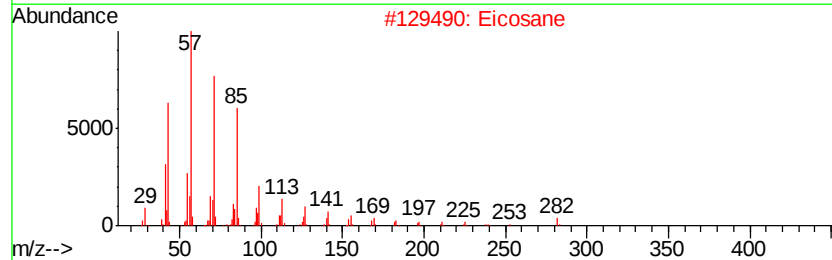
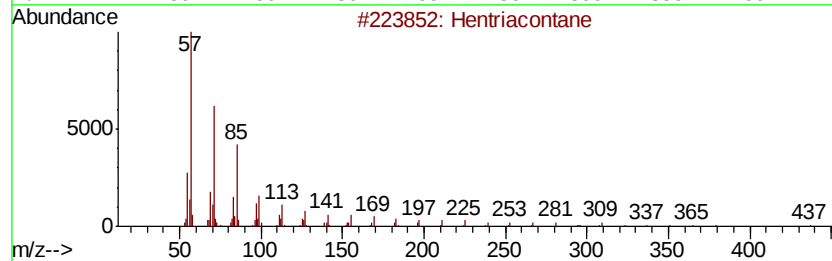
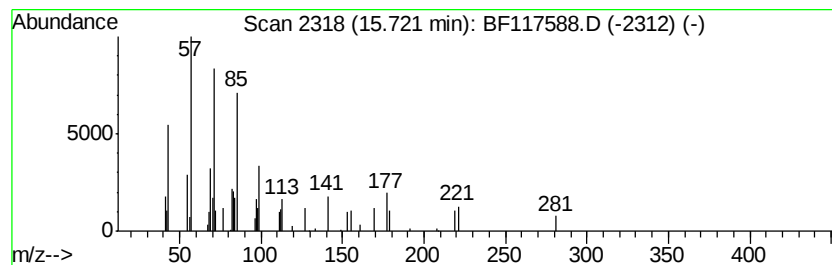
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	3.24 ng	35950	Perylene-d12	15.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hentriacontane	437	C31H64	000630-04-6	90
2		Eicosane	282	C20H42	000112-95-8	90
3		Pentacosane	352	C25H52	000629-99-2	90
4		Heptacosane	380	C27H56	000593-49-7	86
5		Heneicosane	296	C21H44	000629-94-7	86



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Acq On : 29 Oct 2019 14:04
Operator : JU
Sample : K5503-15
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
172-22-(0-2)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.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
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unknown6.50	6.50	81.5	ng	921199	1	6.73	226011	20.0
unknown11.77	11.77	2.7	ng	25723	4	11.25	187950	20.0
Octacosyl trifluo...	13.73	7.6	ng	97392	5	13.89	257136	20.0
Heneicosane	14.34	2.4	ng	31062	5	13.89	257136	20.0
Naphthalene, 1-(2...	14.40	5.3	ng	67655	5	13.89	257136	20.0
Eicosane	14.64	4.2	ng	46551	6	15.33	221654	20.0
Squalene	14.71	3.1	ng	34432	6	15.33	221654	20.0
Hentriacontane	15.72	3.2	ng	35950	6	15.33	221654	20.0