

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112119\
 Data File : BF117915.D
 Acq On : 21 Nov 2019 16:33
 Operator : JU
 Sample : K5904-02
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 1-(4-6)

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-BF111319.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	2.175	10	15	27	rVB	758452	1108540	17.56%	2.441%
2	5.128	512	517	526	rVB	548056	690212	10.94%	1.520%
3	5.534	580	586	589	rBV	3347639	3471855	55.01%	7.646%
4	6.539	752	757	760	rBV	3905810	4107390	65.08%	9.046%
5	6.686	777	782	785	rBV	4720565	4357685	69.05%	9.597%
6	6.916	817	821	824	rBV	1114984	860400	13.63%	1.895%
7	7.075	844	848	851	rBV	4058336	3436151	54.45%	7.568%
8	7.481	912	917	920	rBV	2887530	2702739	42.82%	5.953%
9	8.204	1036	1040	1043	rBV	1329809	1122649	17.79%	2.473%
10	9.280	1219	1223	1227	rBV	5363645	4962793	78.64%	10.930%
11	9.674	1286	1290	1294	rBV	800656	648367	10.27%	1.428%
12	9.963	1336	1339	1348	rVB	1526189	1390816	22.04%	3.063%
13	10.757	1470	1474	1477	rBV	3819349	3411376	54.05%	7.513%
14	11.457	1589	1593	1597	rBV	1709995	1475463	23.38%	3.250%
15	11.974	1678	1681	1692	rBV	232352	277436	4.40%	0.611%
16	12.768	1812	1816	1821	rBV	104783	138894	2.20%	0.306%
17	12.857	1827	1831	1834	rVB	80787	77384	1.23%	0.170%
18	13.051	1859	1864	1870	rBV	5984174	6311164	100.00%	13.900%
19	13.945	2012	2016	2025	rBV4	210809	480819	7.62%	1.059%
20	14.104	2039	2043	2047	rVB	1484420	1271871	20.15%	2.801%
21	14.886	2173	2176	2181	rVB	78677	75143	1.19%	0.165%
22	14.968	2185	2190	2194	rBV	960775	974436	15.44%	2.146%
23	15.239	2232	2236	2240	rBV	109380	123581	1.96%	0.272%
24	15.615	2294	2300	2303	rBV	1017703	1353958	21.45%	2.982%
25	16.098	2378	2382	2389	rVB	119744	185386	2.94%	0.408%
26	16.633	2468	2473	2480	rVB2	92218	158478	2.51%	0.349%
27	17.262	2575	2580	2586	rVB	61968	127127	2.01%	0.280%
28	18.003	2702	2706	2716	rVB4	43316	102602	1.63%	0.226%

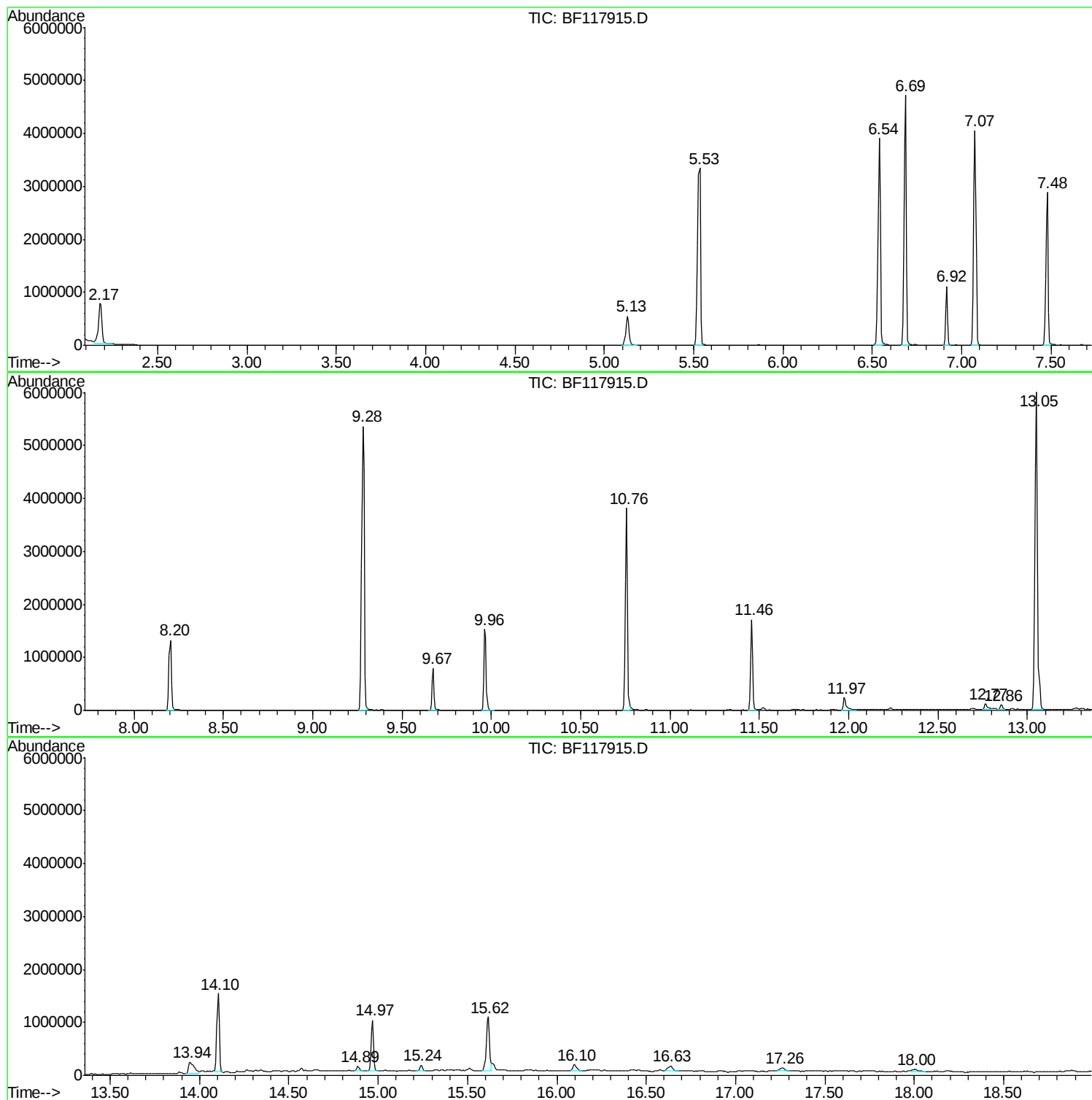
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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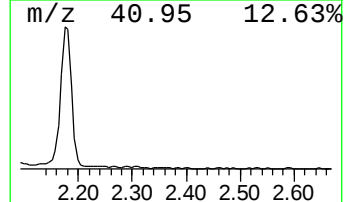
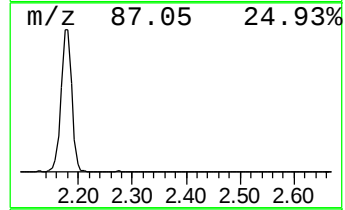
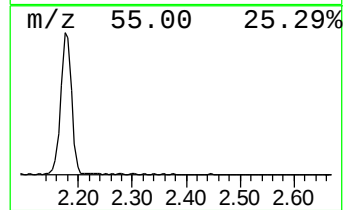
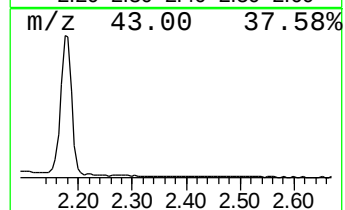
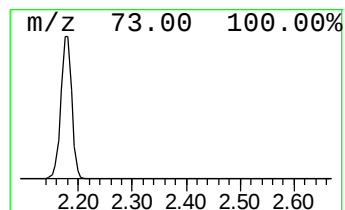
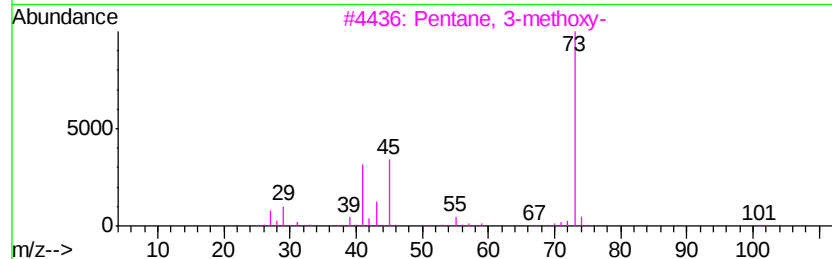
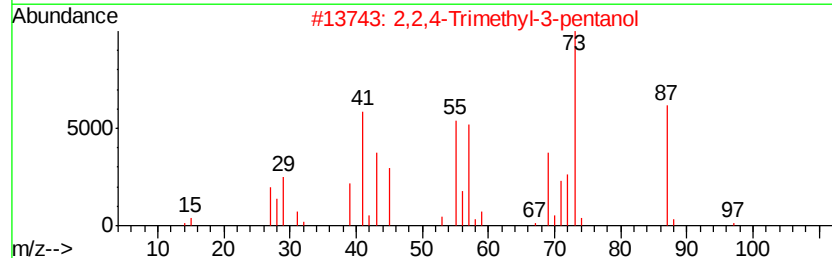
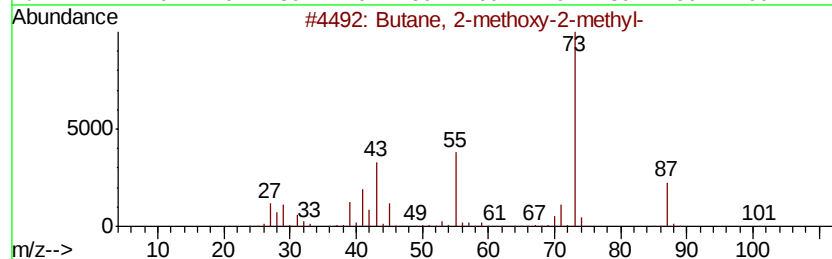
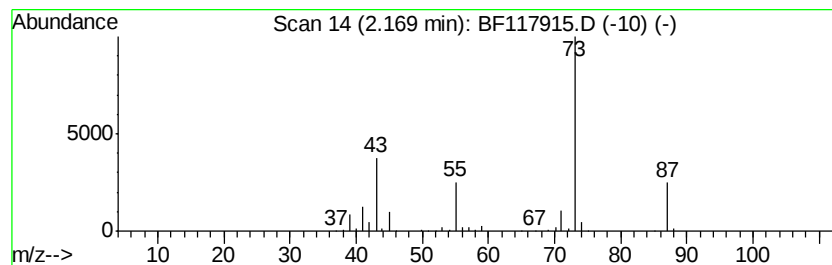
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.17	25.77 ng	1108540	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	56
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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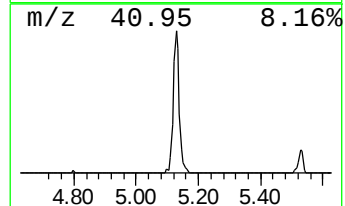
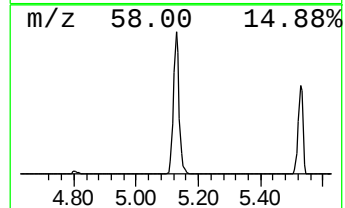
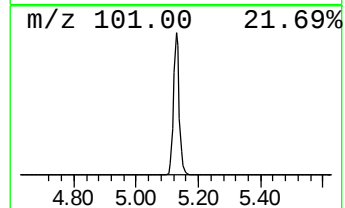
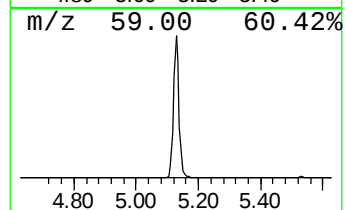
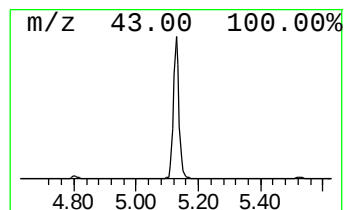
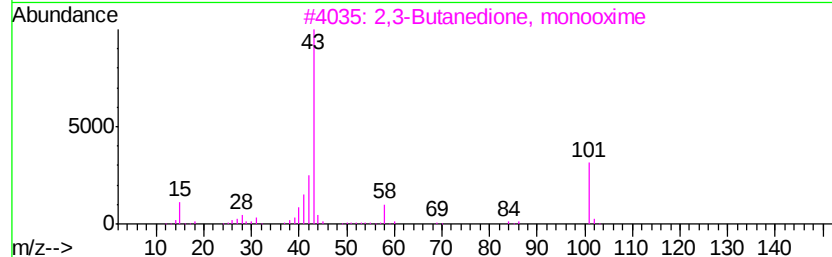
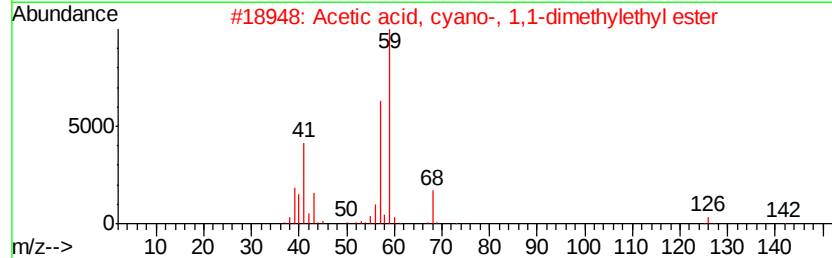
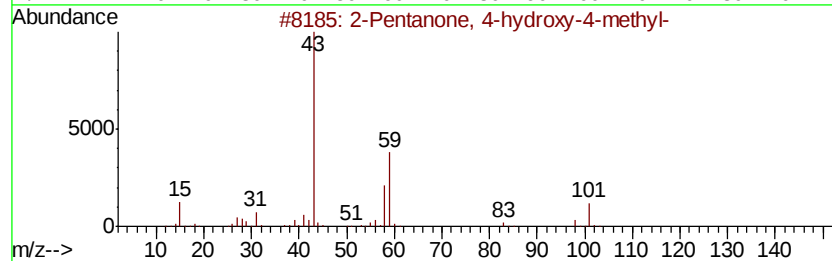
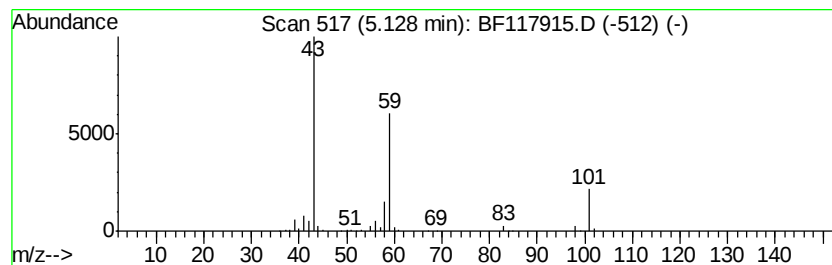
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	16.04 ng	690212	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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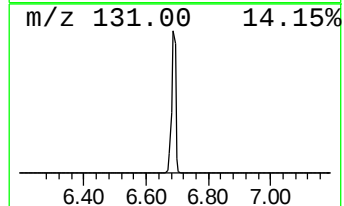
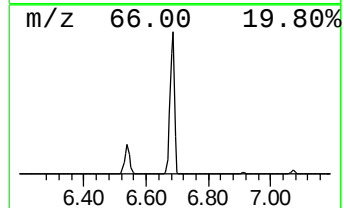
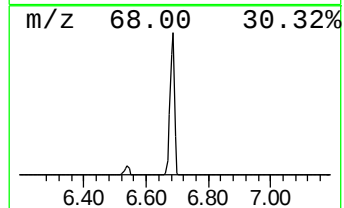
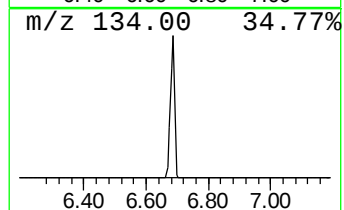
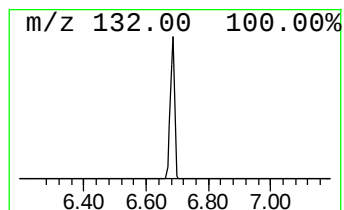
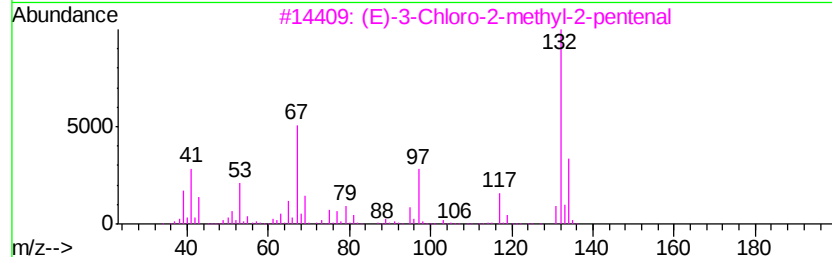
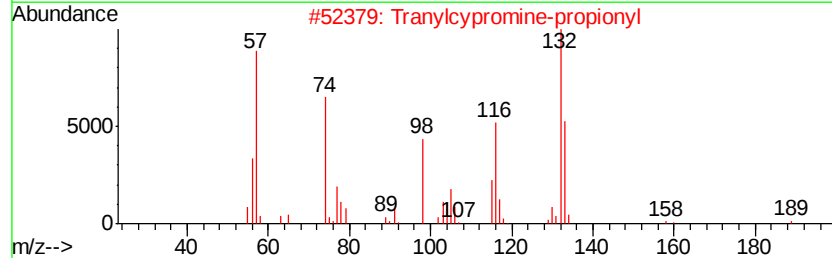
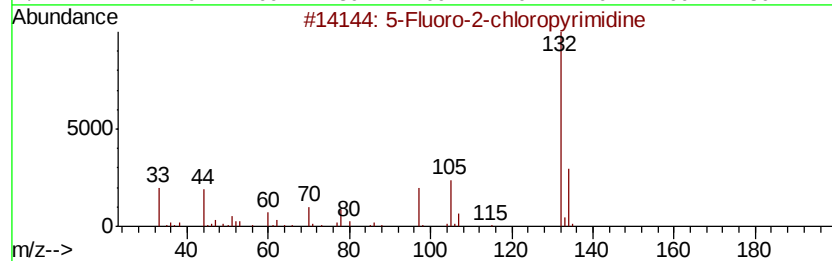
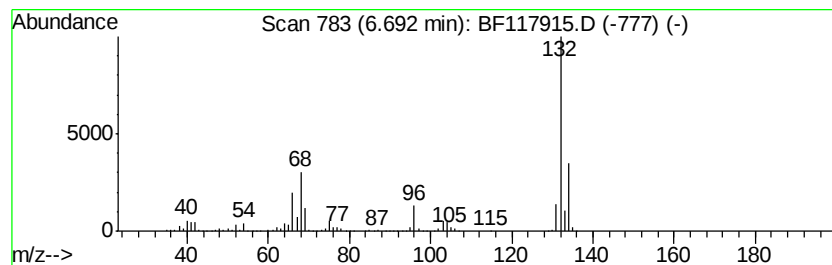
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	101.29 ng	4357690	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranlycypropine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
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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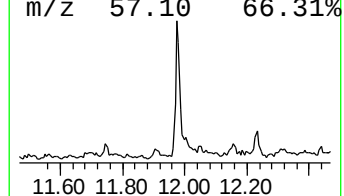
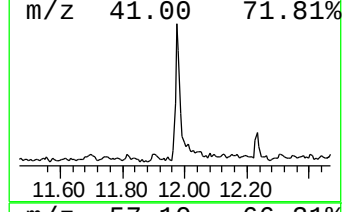
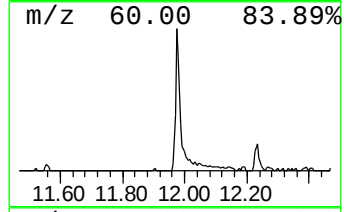
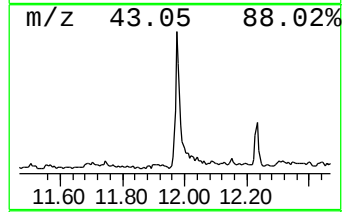
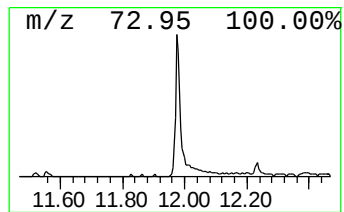
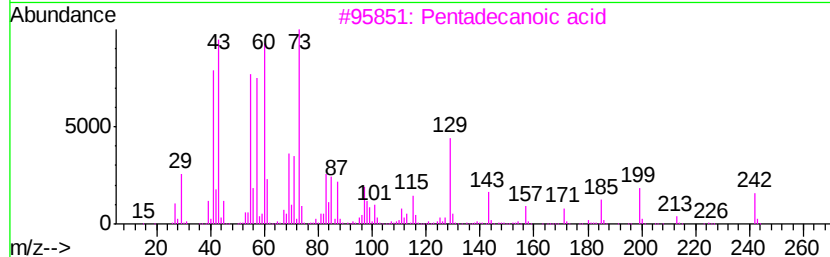
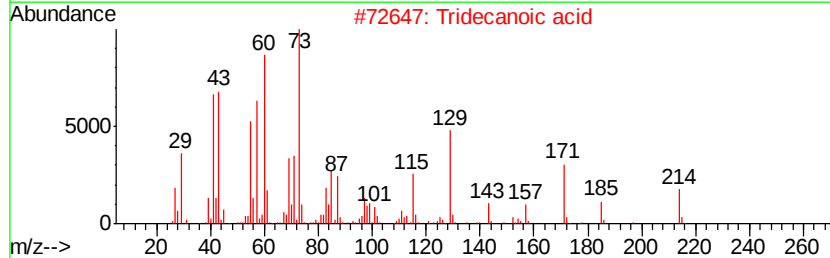
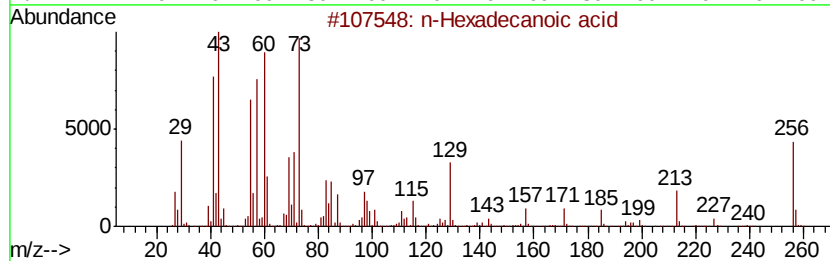
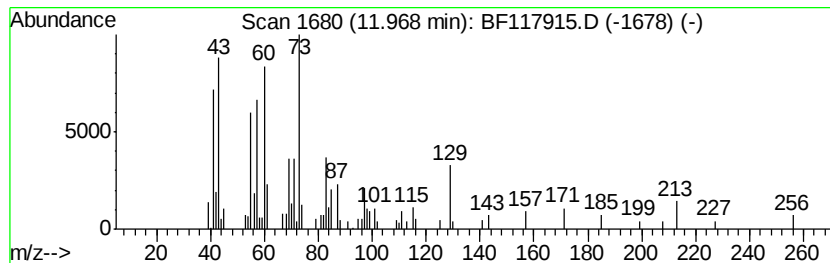
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.97	3.76 ng	277436	Phenanthrene-d10	11.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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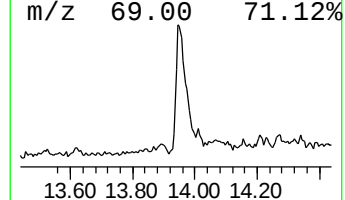
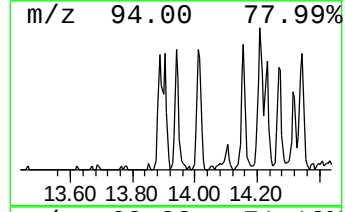
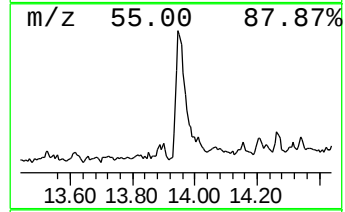
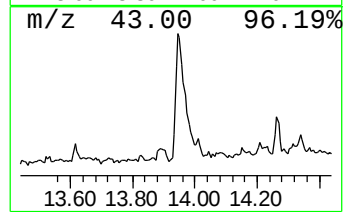
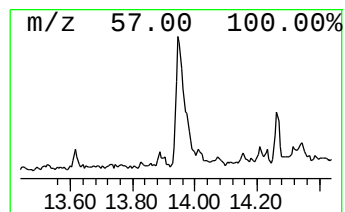
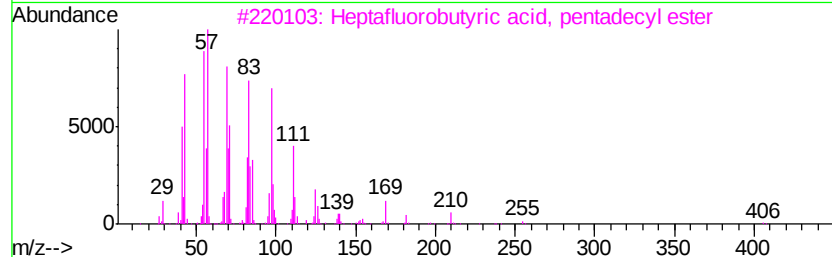
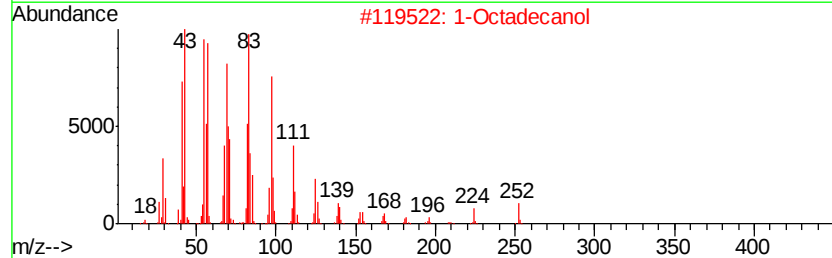
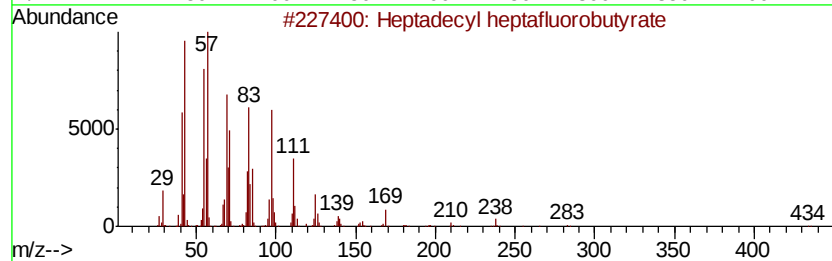
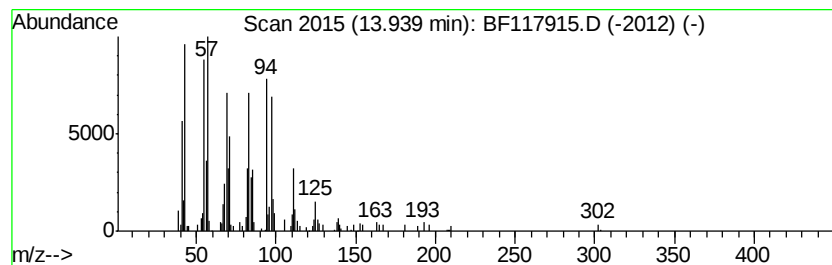
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	7.56 ng	480819	Chrysene-d12	14.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	93
2		1-Octadecanol	270	C18H38O	000112-92-5	92
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87



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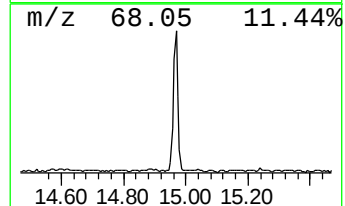
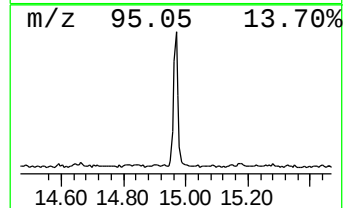
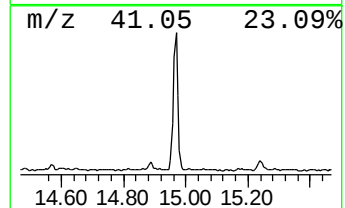
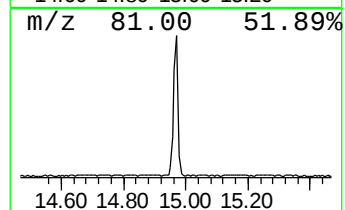
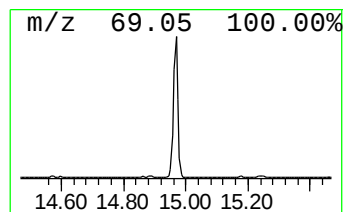
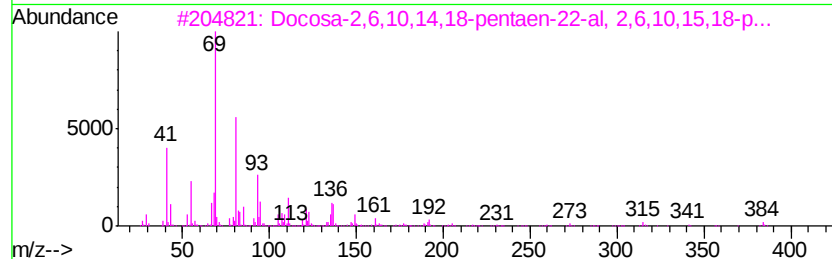
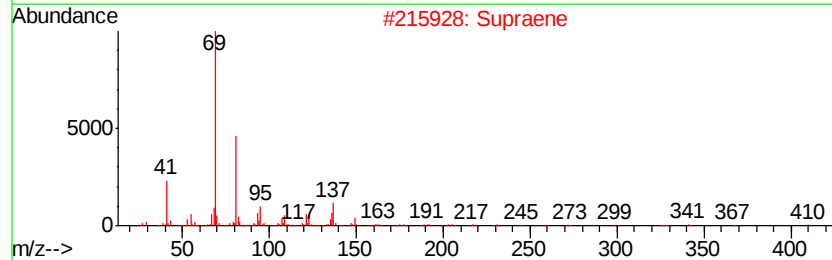
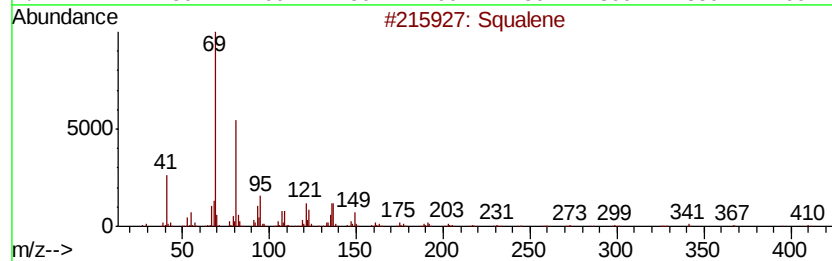
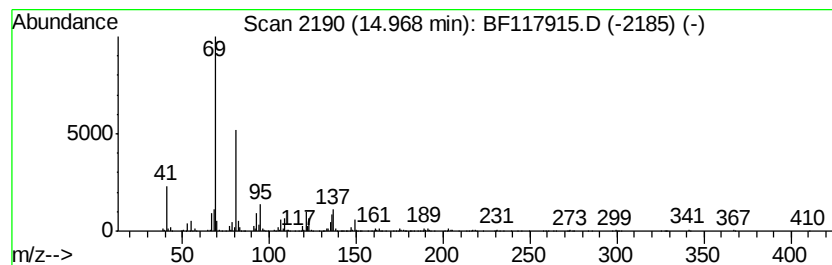
Instrument :
BNA_F
ClientSampleId :
1-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.97	14.39 ng	974436	Perylene-d12	15.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	95
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	90
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117915.D
Acq On : 21 Nov 2019 16:33
Operator : JU
Sample : K5904-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-(4-6)

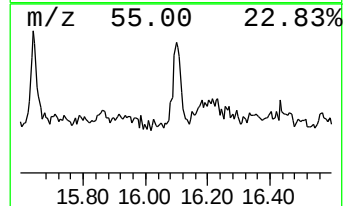
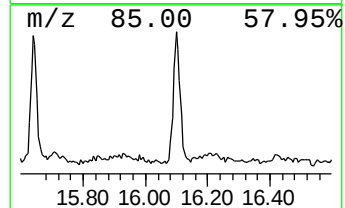
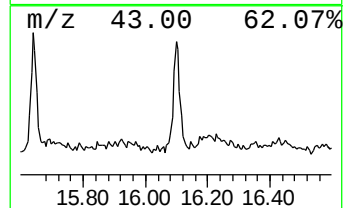
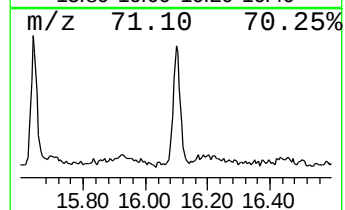
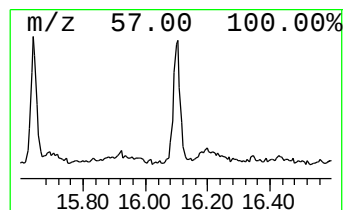
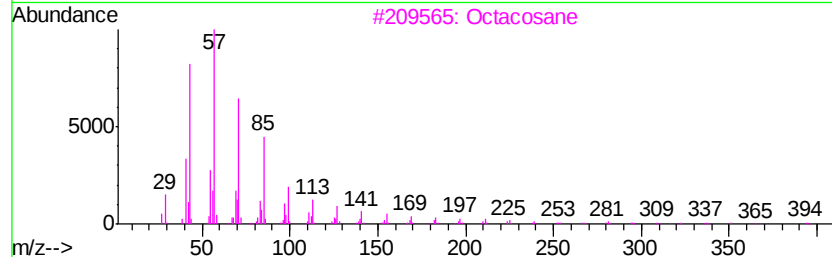
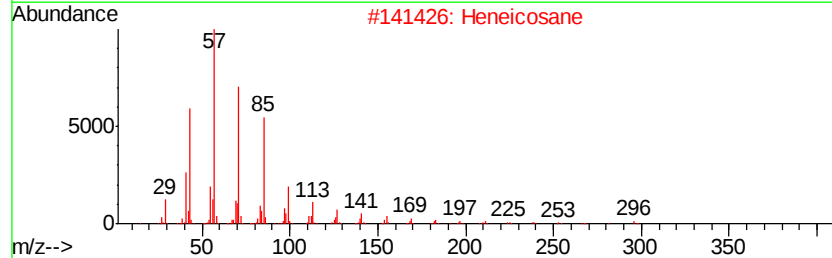
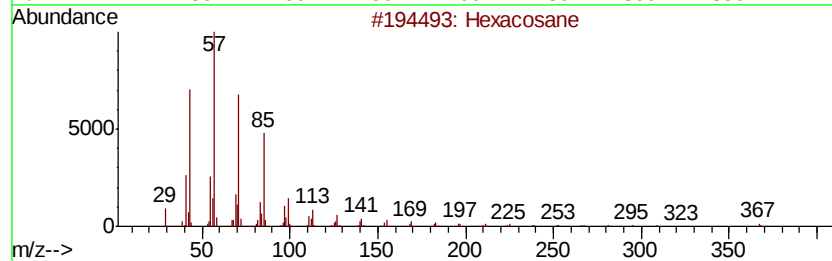
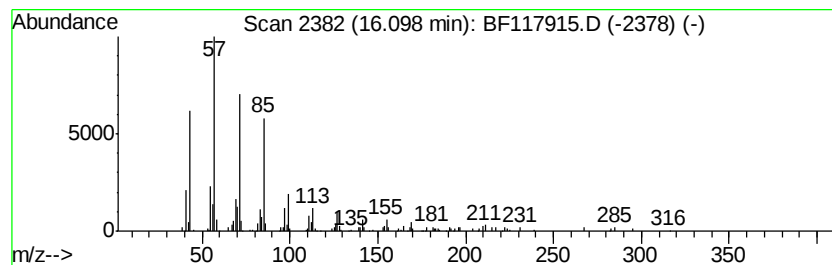
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.10	2.74 ng	185386	Perylene-d12	15.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112119\
Data File : BF117915.D
Acq On : 21 Nov 2019 16:33
Operator : JU
Sample : K5904-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-(4-6)

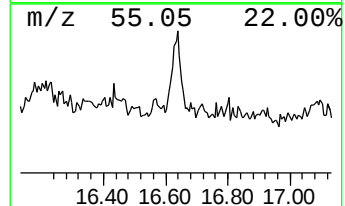
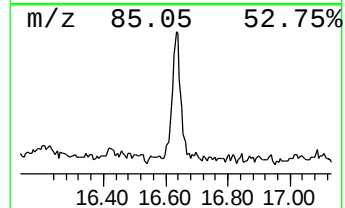
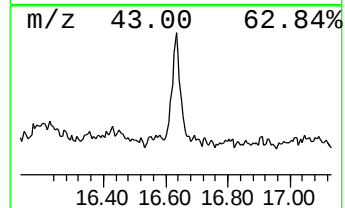
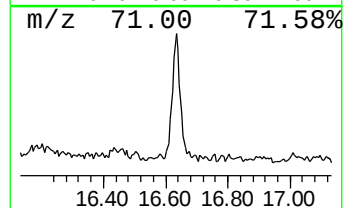
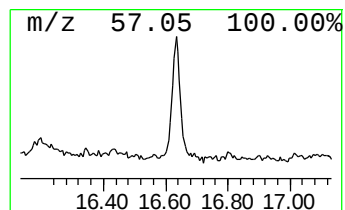
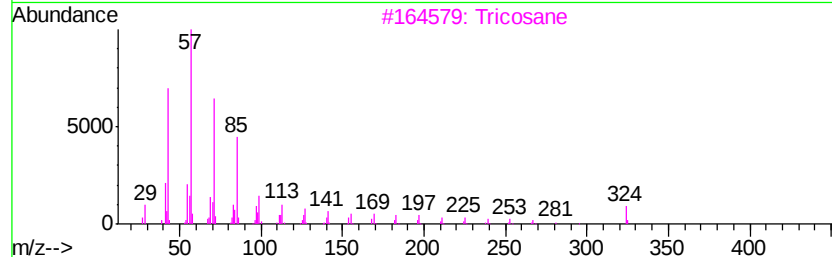
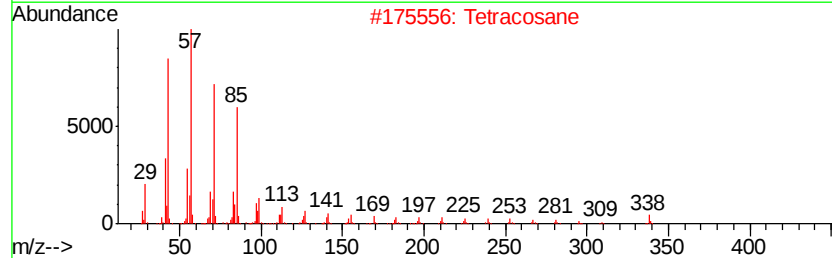
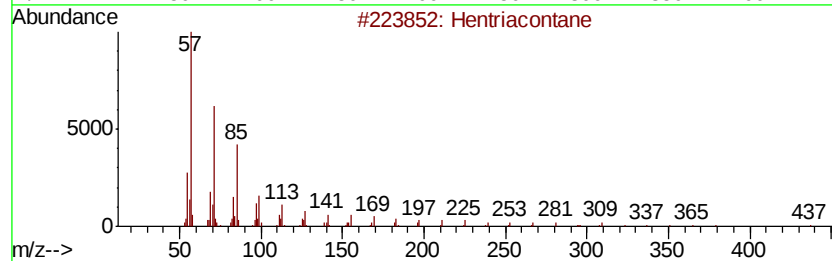
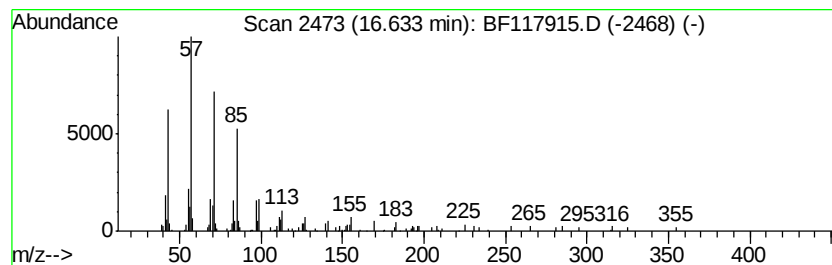
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.34 ng	158478	Perylene-d12	15.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	93
2	Tetracosane		338	C24H50	000646-31-1	91
3	Tricosane		324	C23H48	000638-67-5	91
4	Tetratetracontane		619	C44H90	007098-22-8	90
5	2-methyloctacosane		408	C29H60	1000376-72-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112119\
Data File : BF117915.D
Acq On : 21 Nov 2019 16:33
Operator : JU
Sample : K5904-02
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1-(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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...	2.17	25.8	ng	1108540	1	6.92	860400	20.0
2-Pentanone, 4-hy...	5.13	16.0	ng	690212	1	6.92	860400	20.0
unknown6.69	6.69	101.3	ng	4357690	1	6.92	860400	20.0
n-Hexadecanoic acid	11.97	3.8	ng	277436	4	11.46	1475460	20.0
Heptadecyl hepta...	13.94	7.6	ng	480819	5	14.10	1271870	20.0
Squalene	14.97	14.4	ng	974436	6	15.62	1353960	20.0
Hexacosane	16.10	2.7	ng	185386	6	15.62	1353960	20.0
Hentriacontane	16.63	2.3	ng	158478	6	15.62	1353960	20.0