

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
 Data File : BF112449.D
 Acq On : 7 Feb 2019 20:16
 Operator : JU/SJ
 Sample : K1385-06
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 98-SB-01-4-57

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-BF012519.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	2.128	3	7	22	rVB	119212	176744	4.02%	0.506%
2	4.440	396	400	408	rBV	38957	57065	1.30%	0.163%
3	5.063	502	506	518	rBV	121909	182270	4.15%	0.522%
4	5.475	572	576	595	rBV	3610005	3594630	81.81%	10.292%
5	6.486	743	748	765	rBV	3403154	3920011	89.21%	11.224%
6	6.610	765	769	778	rVV	4077582	3973182	90.42%	11.376%
7	6.834	803	807	815	rBV	859776	763110	17.37%	2.185%
8	6.992	829	834	837	rBV	3279888	3100179	70.55%	8.877%
9	7.398	898	903	906	rBV	2475874	2310616	52.59%	6.616%
10	8.116	1021	1025	1038	rBV	979487	952957	21.69%	2.729%
11	9.186	1202	1207	1211	rBV	4416669	4394057	100.00%	12.581%
12	9.580	1270	1274	1284	rBV	216840	203269	4.63%	0.582%
13	9.869	1319	1323	1337	rVB	1201029	1069320	24.34%	3.062%
14	10.663	1454	1458	1473	rBV	2737026	2590010	58.94%	7.416%
15	11.357	1572	1576	1585	rBV	1083252	1018506	23.18%	2.916%
16	11.880	1659	1665	1673	rBV3	151985	212325	4.83%	0.608%
17	12.574	1780	1783	1788	rBV	40354	46537	1.06%	0.133%
18	12.663	1795	1798	1804	rBV4	44859	57380	1.31%	0.164%
19	12.739	1808	1811	1816	rVB	91977	93027	2.12%	0.266%
20	12.939	1840	1845	1848	rBV	4035112	3536142	80.48%	10.125%
21	13.410	1920	1925	1931	rBV	436300	438780	9.99%	1.256%
22	13.827	1991	1996	2003	rBV	151162	198329	4.51%	0.568%
23	14.004	2022	2026	2033	rVB	831247	839225	19.10%	2.403%
24	14.451	2098	2102	2107	rBV	63302	68977	1.57%	0.198%
25	14.751	2148	2153	2158	rBV3	73486	100035	2.28%	0.286%
26	14.833	2164	2167	2170	rVB	74042	72757	1.66%	0.208%
27	15.086	2206	2210	2214	rVB	75422	85021	1.93%	0.243%
28	15.474	2270	2276	2284	rBV	532362	809566	18.42%	2.318%
29	15.886	2343	2346	2352	rVB	44678	60817	1.38%	0.174%

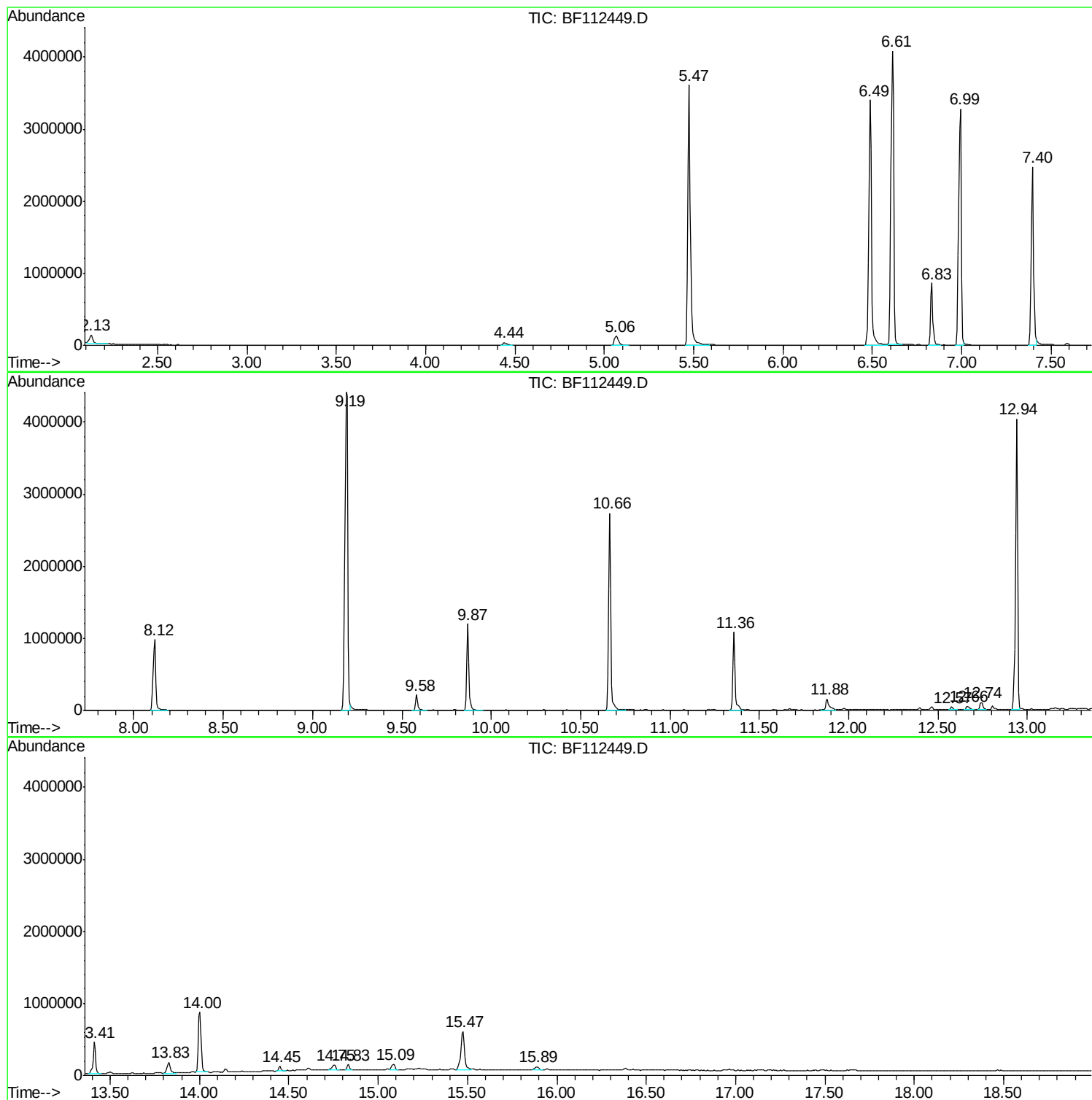
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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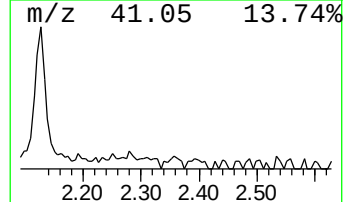
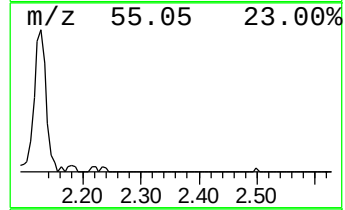
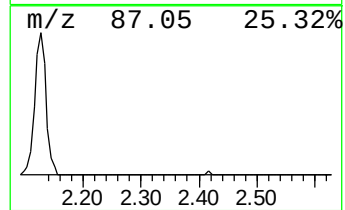
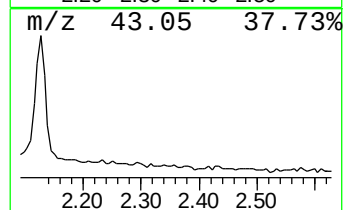
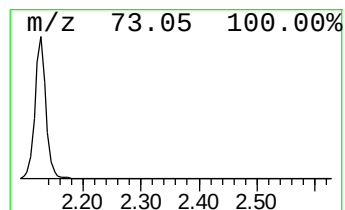
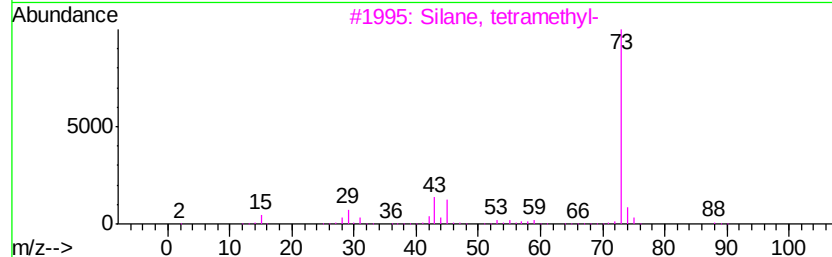
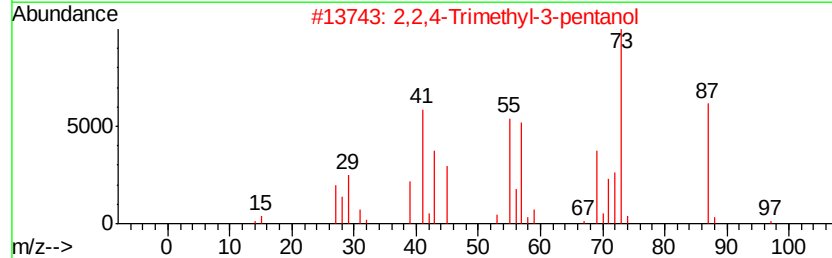
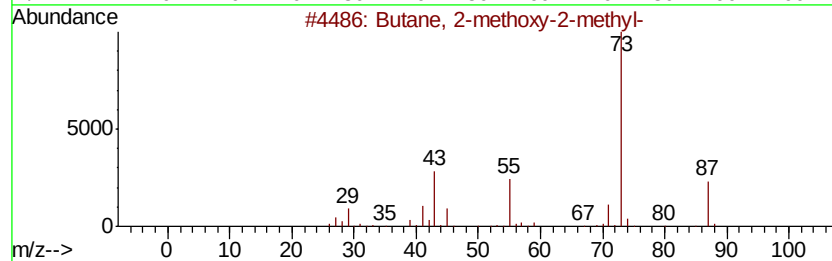
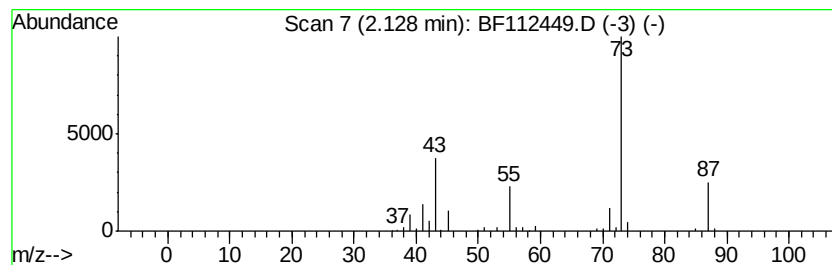
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.13	4.63 ng	176744	1,4-Dichlorobenzene-d4	6.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	16



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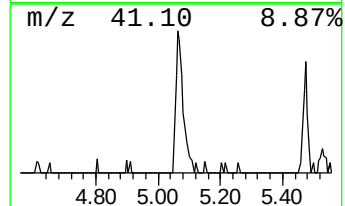
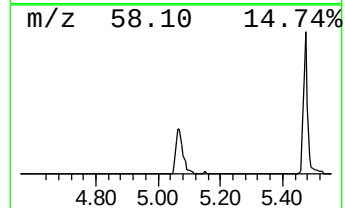
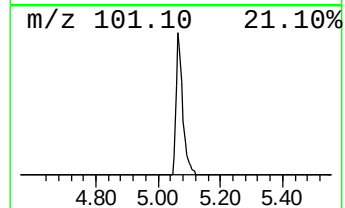
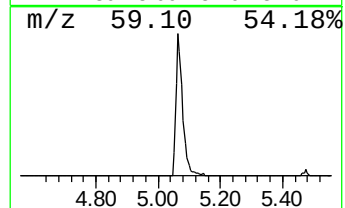
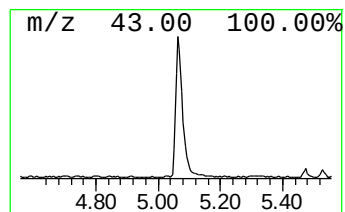
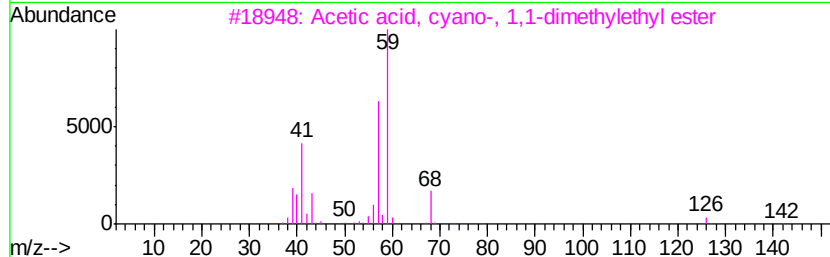
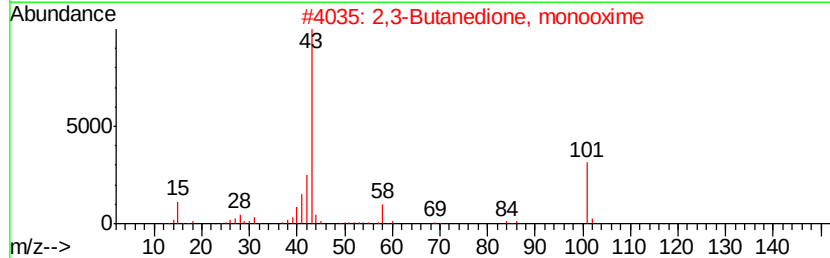
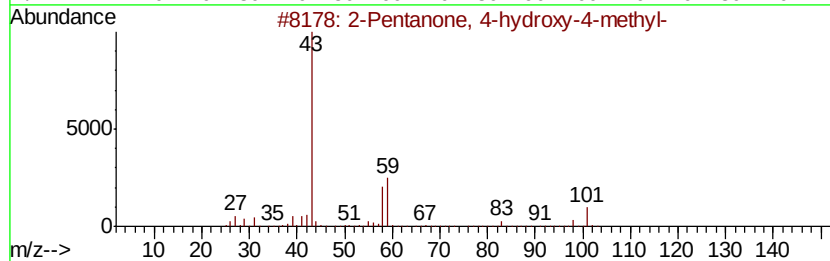
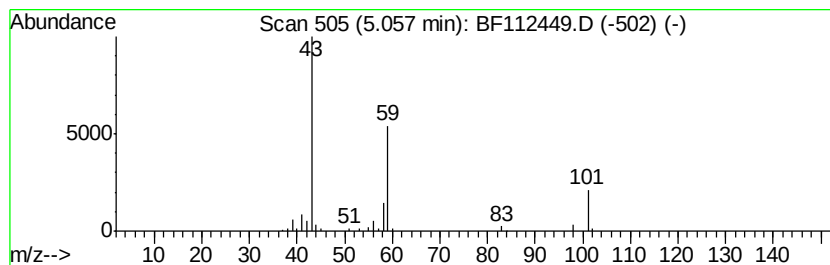
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	4.78 ng	182270	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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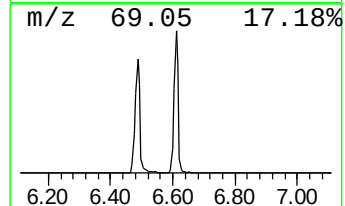
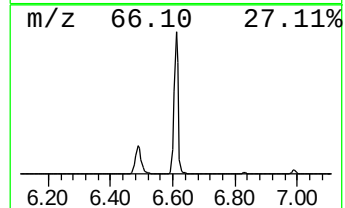
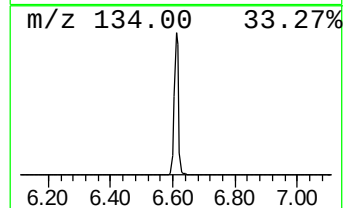
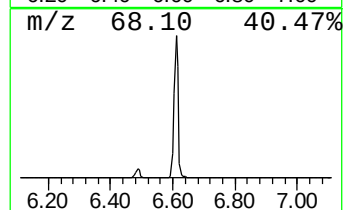
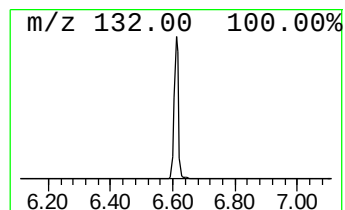
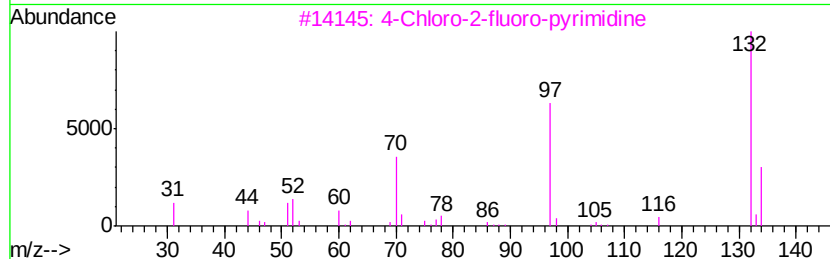
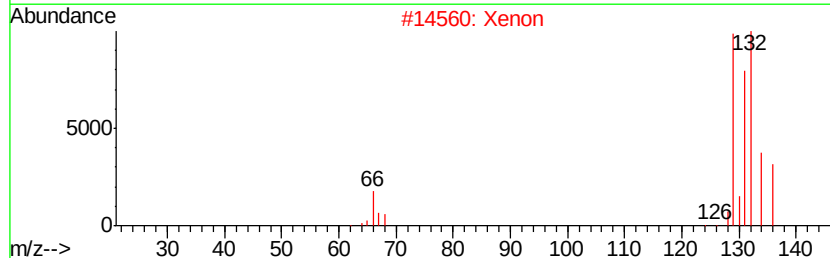
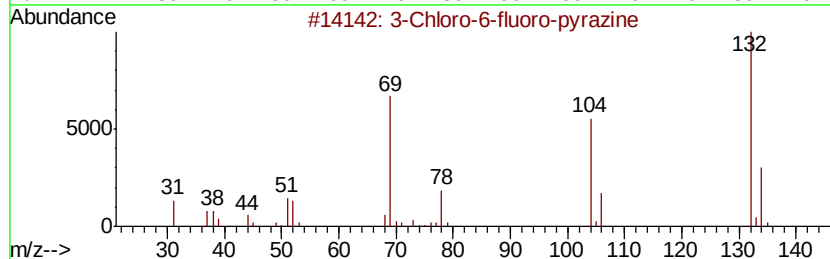
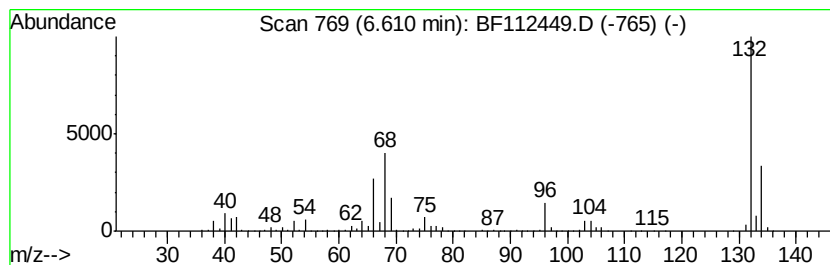
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Peak Number 3 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	104.13 ng	3973180	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Xenon	132	Xe	007440-63-3	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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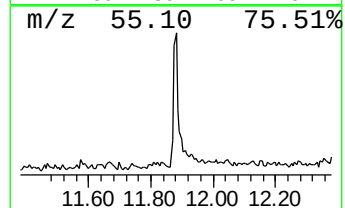
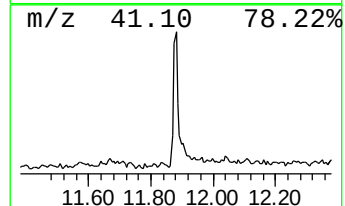
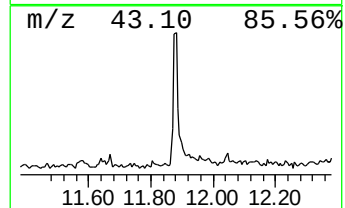
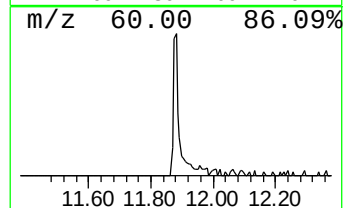
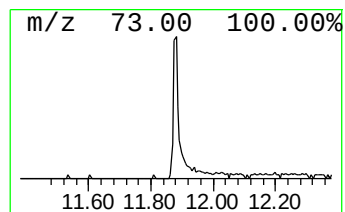
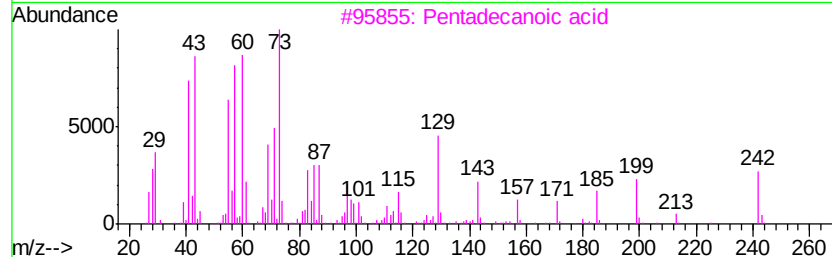
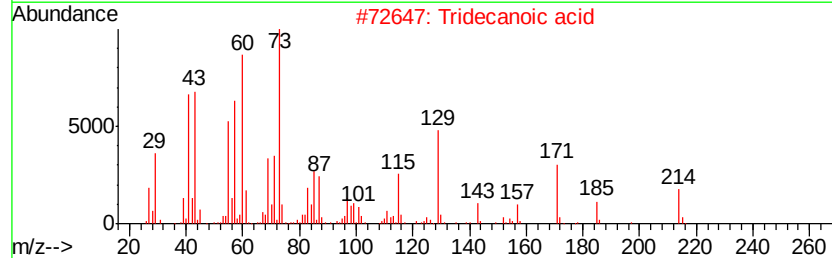
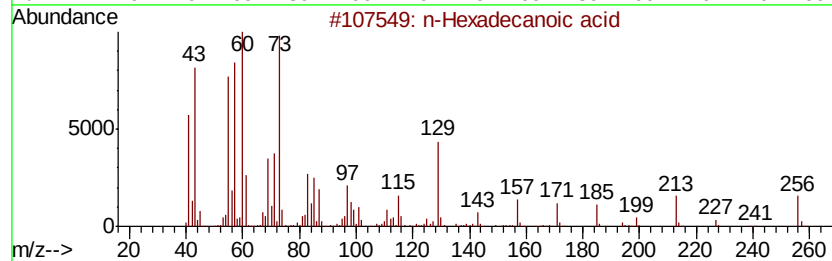
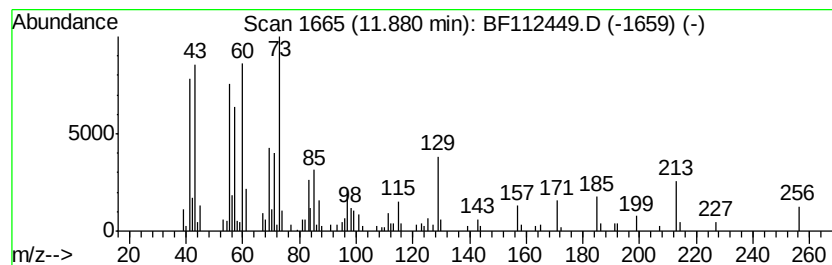
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.88	4.17 ng	212325	Phenanthrene-d10		11.36	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4		n-Decanoic acid	172	C10H20O2	000334-48-5	62
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	62



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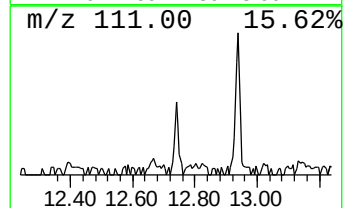
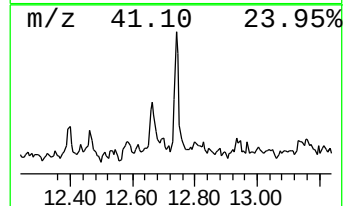
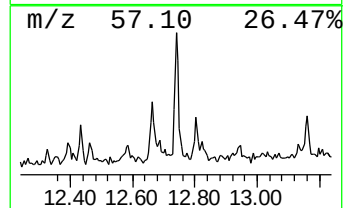
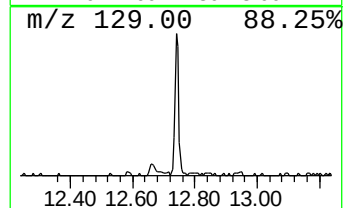
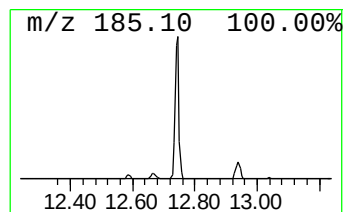
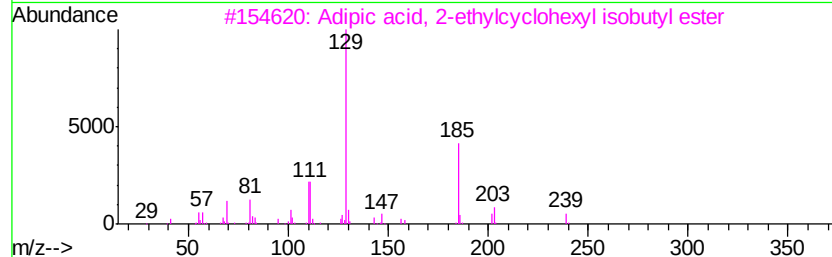
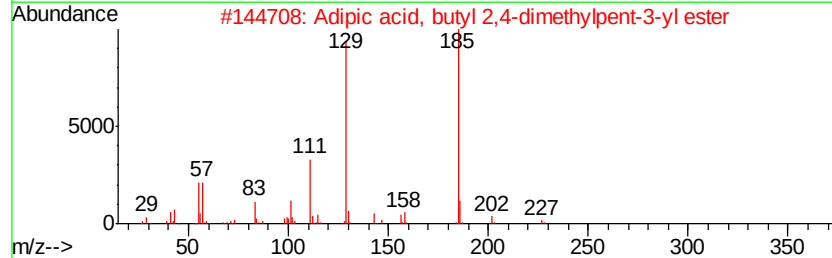
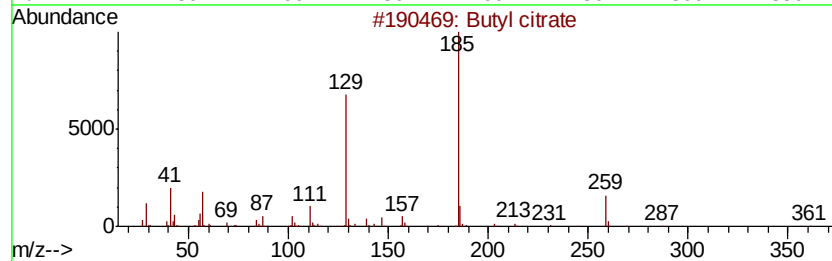
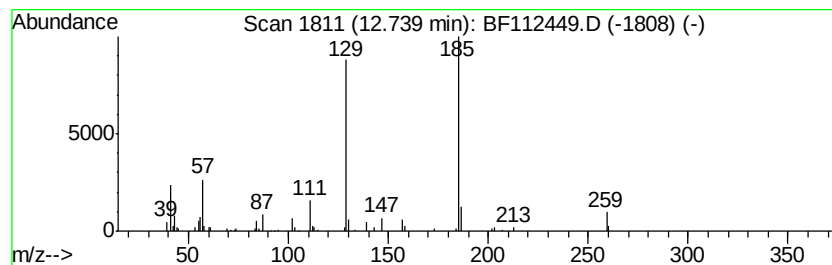
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Peak Number 6 Butyl citrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.22 ng	93027	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butyl citrate	360 C18H32O7	000077-94-1	91
2	Adipic acid, butyl 2,4-dimethylp...	300 C17H32O4	1000349-77-7	72
3	Adipic acid, 2-ethylcyclohexyl i...	312 C18H32O4	1000324-22-5	72
4	Adipic acid, 2,4-dimethylpent-3-...	300 C17H32O4	1000349-77-6	64
5	O-Methyl-DL-serine, N-dimethylam...	230 C11H22N2O3	1000375-99-5	64



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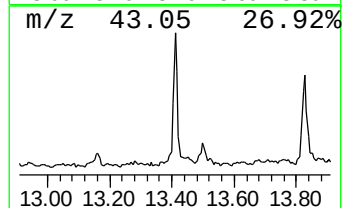
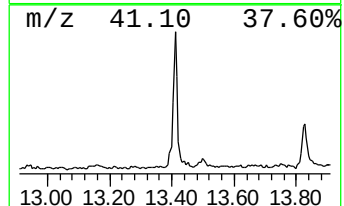
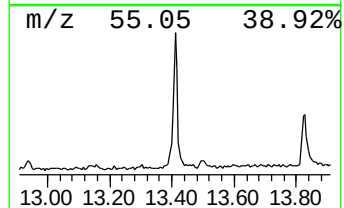
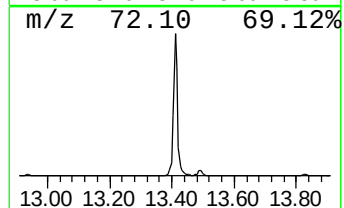
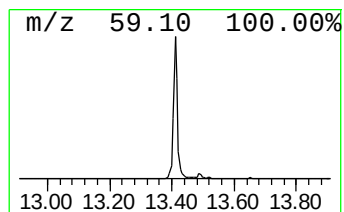
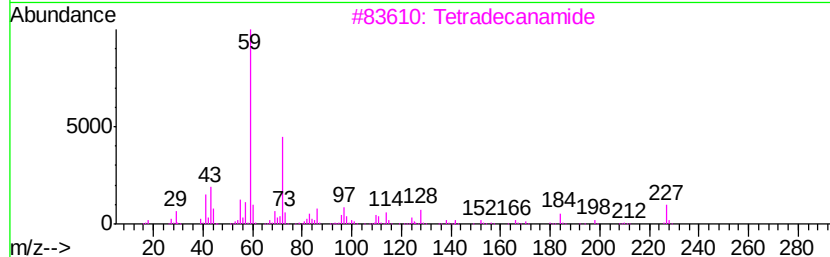
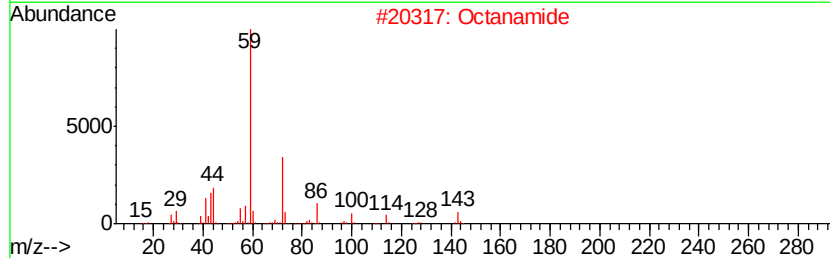
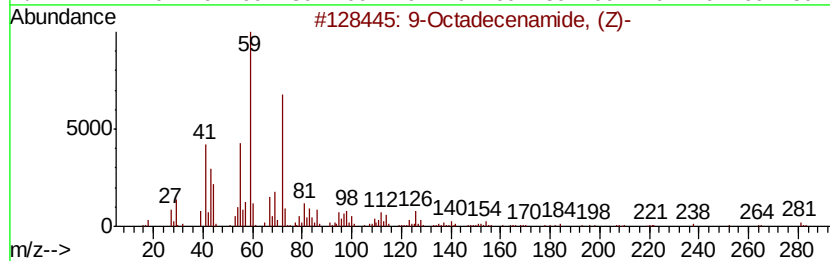
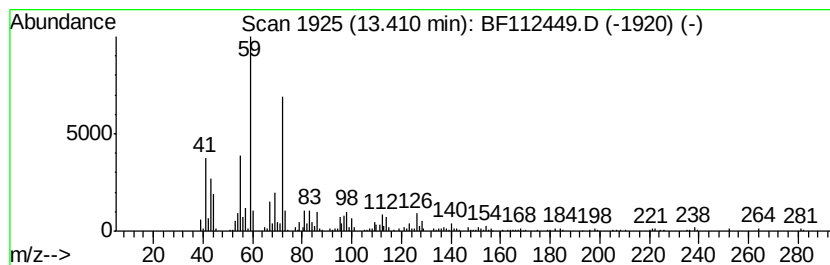
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	10.46 ng	438780	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	95
2		Octanamide	143	C8H17NO	000629-01-6	59
3		Tetradecanamide	227	C14H29NO	000638-58-4	50
4		4-Cyclohexylbutyramide	169	C10H19NO	004441-62-7	45
5		Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	43



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112449.D
Acq On : 7 Feb 2019 20:16
Operator : JU/SJ
Sample : K1385-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

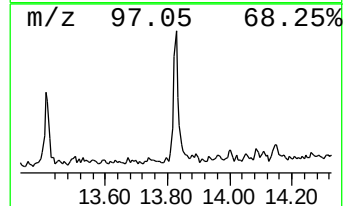
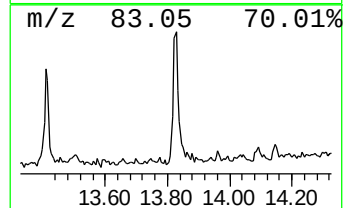
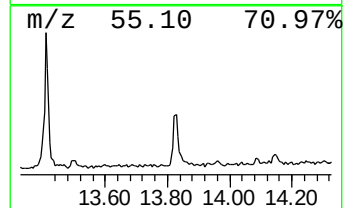
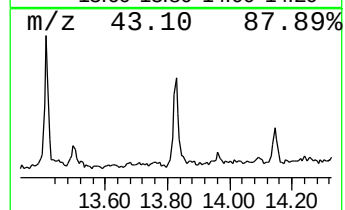
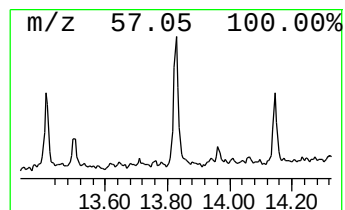
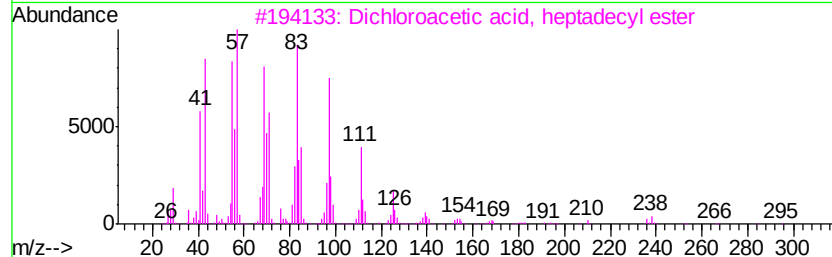
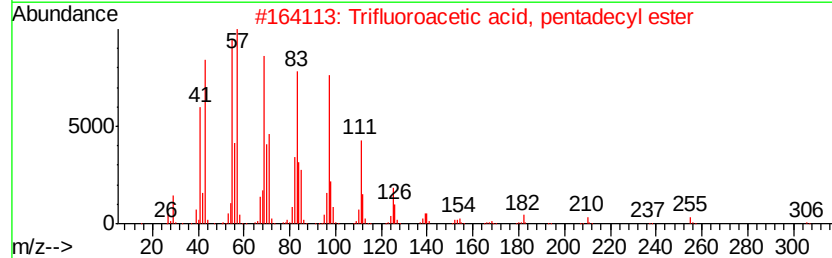
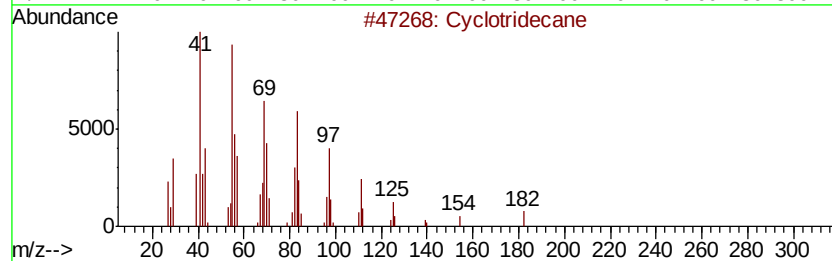
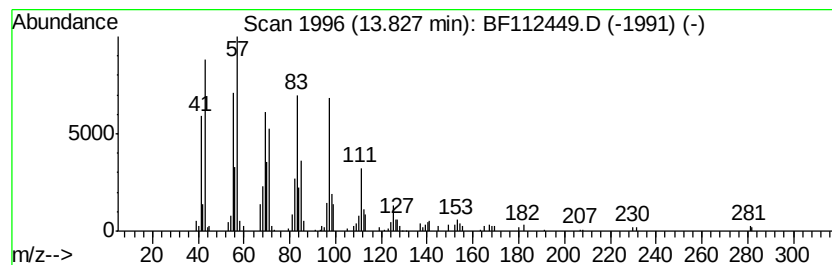
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98-SB-01-4-57

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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 Cyclotridecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.73 ng	198329	Chrysene-d12	14.00
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclotridecane	182 C13H26	000295-02-3 95
2		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 93
3		Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2 91
4		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 91
5		Pentafluoropropionic acid, hexad...	388 C19H33F5O2	006222-07-7 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112449.D
Acq On : 7 Feb 2019 20:16
Operator : JU/SJ
Sample : K1385-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
98-SB-01-4-57

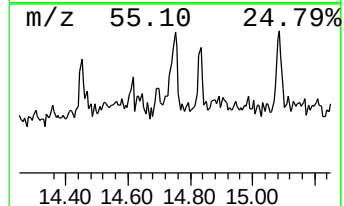
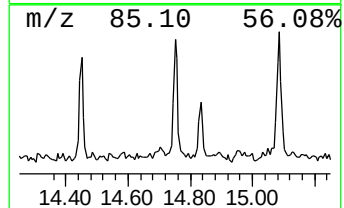
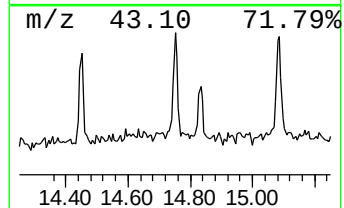
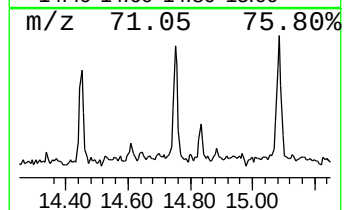
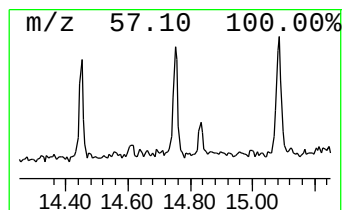
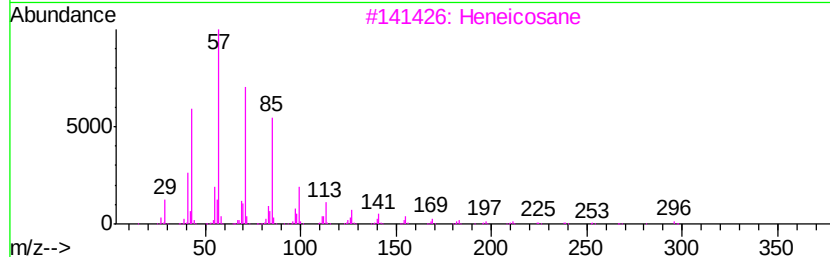
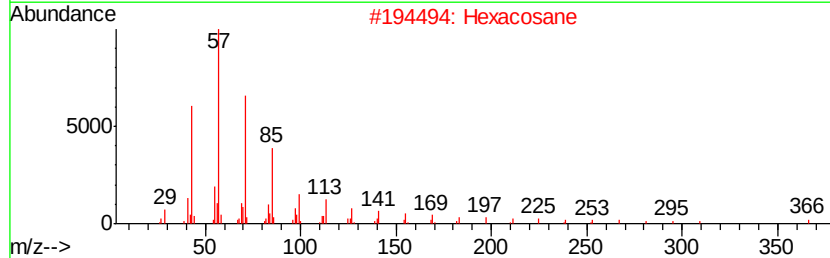
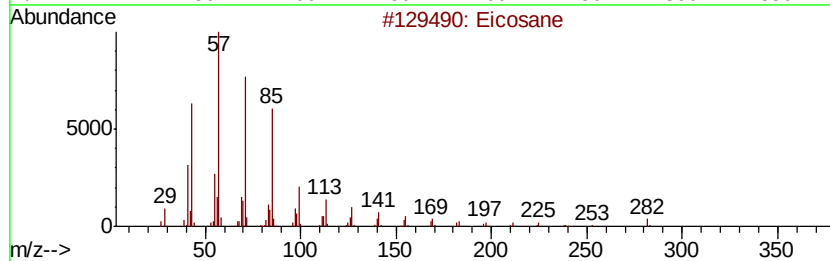
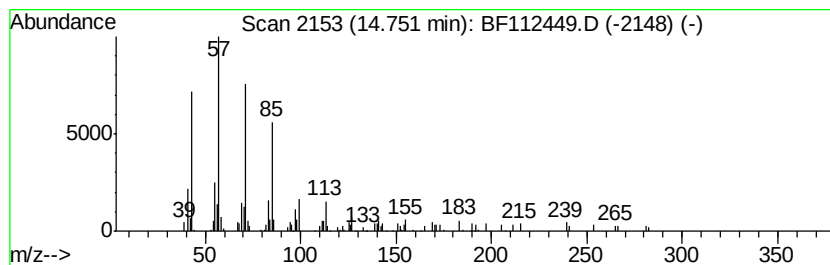
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.75	2.47 ng	100035	Perylene-d12	15.47

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	97
2	Hexacosane		366	C26H54	000630-01-3	91
3	Heneicosane		296	C21H44	000629-94-7	90
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	87
5	Octacosane		394	C28H58	000630-02-4	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020719\
Data File : BF112449.D
Acq On : 7 Feb 2019 20:16
Operator : JU/SJ
Sample : K1385-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

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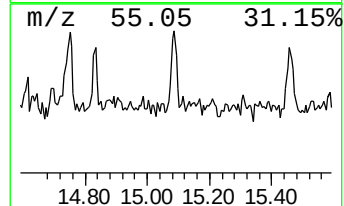
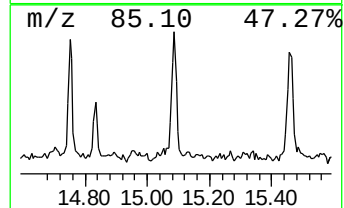
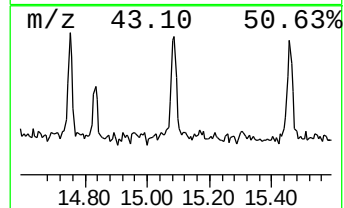
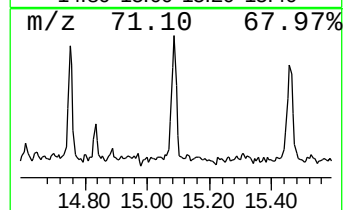
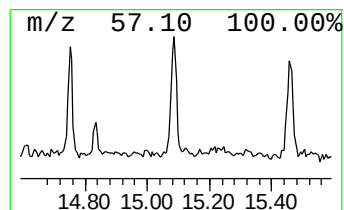
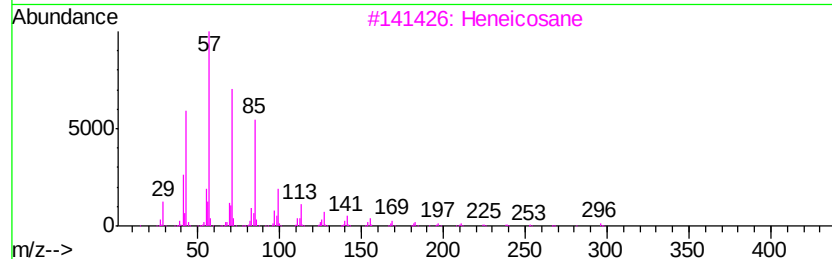
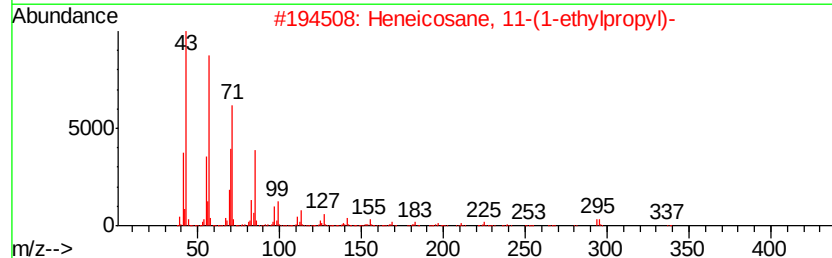
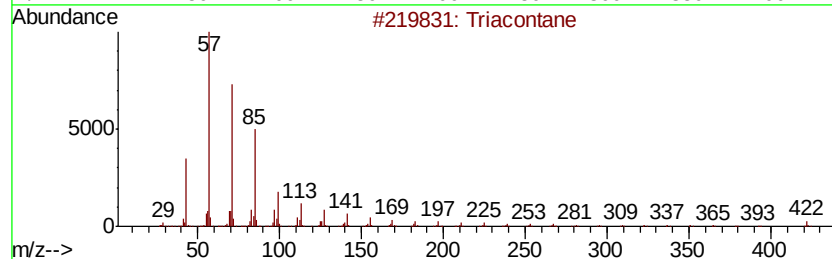
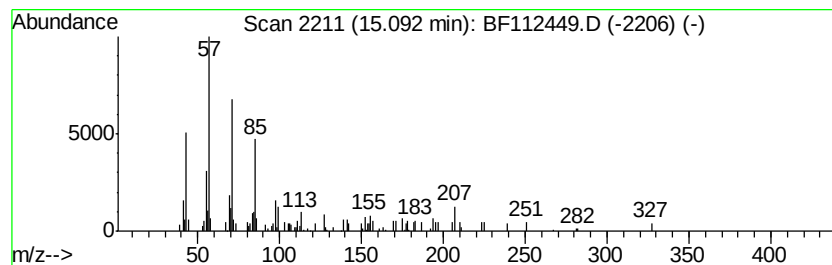
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Triacontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	2.10 ng	85021	Perylene-d12	15.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
3		Heneicosane	296	C21H44	000629-94-7	90
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	90
5		Docosane	310	C22H46	000629-97-0	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020719\
Data File : BF112449.D
Acq On : 7 Feb 2019 20:16
Operator : JU/SJ
Sample : K1385-06
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012519.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...	2.13	4.6	ng	176744	1	6.83	763110	20.0
2-Pentanone, 4-hy...	5.06	4.8	ng	182270	1	6.83	763110	20.0
unknown6.61	6.61	104.1	ng	3973180	1	6.83	763110	20.0
n-Hexadecanoic acid	11.88	4.2	ng	212325	4	11.36	1018510	20.0
Butyl citrate	12.74	2.2	ng	93027	5	14.00	839225	20.0
9-Octadecenamide, ...	13.41	10.5	ng	438780	5	14.00	839225	20.0
Cyclotridecane	13.83	4.7	ng	198329	5	14.00	839225	20.0
Eicosane	14.75	2.5	ng	100035	6	15.47	809566	20.0
Triacontane	15.09	2.1	ng	85021	6	15.47	809566	20.0