

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
 Data File : BF118012.D
 Acq On : 26 Nov 2019 17:32
 Operator : JU
 Sample : K5948-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-1-6-12

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	2.198	11	19	27	rVB	613947	801147	26.12%	2.969%
2	5.110	509	514	525	rVB	434175	552187	18.01%	2.047%
3	5.516	578	583	586	rBV	2585974	2400482	78.28%	8.897%
4	6.522	749	754	757	rBV	2355935	2573064	83.90%	9.537%
5	6.663	774	778	782	rBV	2786250	2674942	87.23%	9.915%
6	6.892	814	817	821	rBV	862384	703297	22.93%	2.607%
7	7.051	840	844	847	rBV	2385241	2051435	66.89%	7.604%
8	7.457	908	913	916	rBV	1994724	1884711	61.46%	6.986%
9	8.180	1032	1036	1040	rBV	1212023	997187	32.52%	3.696%
10	9.263	1215	1220	1223	rBV	3710772	3066671	100.00%	11.366%
11	9.651	1283	1286	1291	rBV	651378	516460	16.84%	1.914%
12	9.945	1332	1336	1340	rBV	1317760	1028633	33.54%	3.813%
13	10.321	1386	1400	1402	rBV5	20275	64044	2.09%	0.237%
14	10.739	1467	1471	1474	rBV	2074379	1757258	57.30%	6.513%
15	11.439	1586	1590	1593	rBV	993259	780477	25.45%	2.893%
16	11.668	1626	1629	1636	rBV2	44447	60831	1.98%	0.225%
17	11.957	1675	1678	1684	rBV	288609	310538	10.13%	1.151%
18	12.392	1746	1752	1754	rBV7	19559	40136	1.31%	0.149%
19	12.663	1795	1798	1801	rBV	37704	54621	1.78%	0.202%
20	12.745	1809	1812	1816	rBV2	102505	108278	3.53%	0.401%
21	12.833	1825	1827	1831	rBV4	24423	40346	1.32%	0.150%
22	12.898	1834	1838	1842	rVV4	60925	75948	2.48%	0.281%
23	13.027	1856	1860	1864	rBV	2816442	2581900	84.19%	9.570%
24	13.251	1894	1898	1901	rBV6	36336	67128	2.19%	0.249%
25	13.721	1975	1978	1979	rBV2	32606	37250	1.21%	0.138%
26	13.933	2011	2014	2020	rVB3	138341	234208	7.64%	0.868%
27	14.092	2037	2041	2048	rVB	670625	622469	20.30%	2.307%
28	14.551	2117	2119	2122	rBV2	57055	44259	1.44%	0.164%
29	14.851	2166	2170	2172	rBV	118151	157915	5.15%	0.585%
30	15.221	2230	2233	2240	rVB	76713	88451	2.88%	0.328%
31	15.598	2292	2297	2306	rBV	381658	603660	19.68%	2.237%

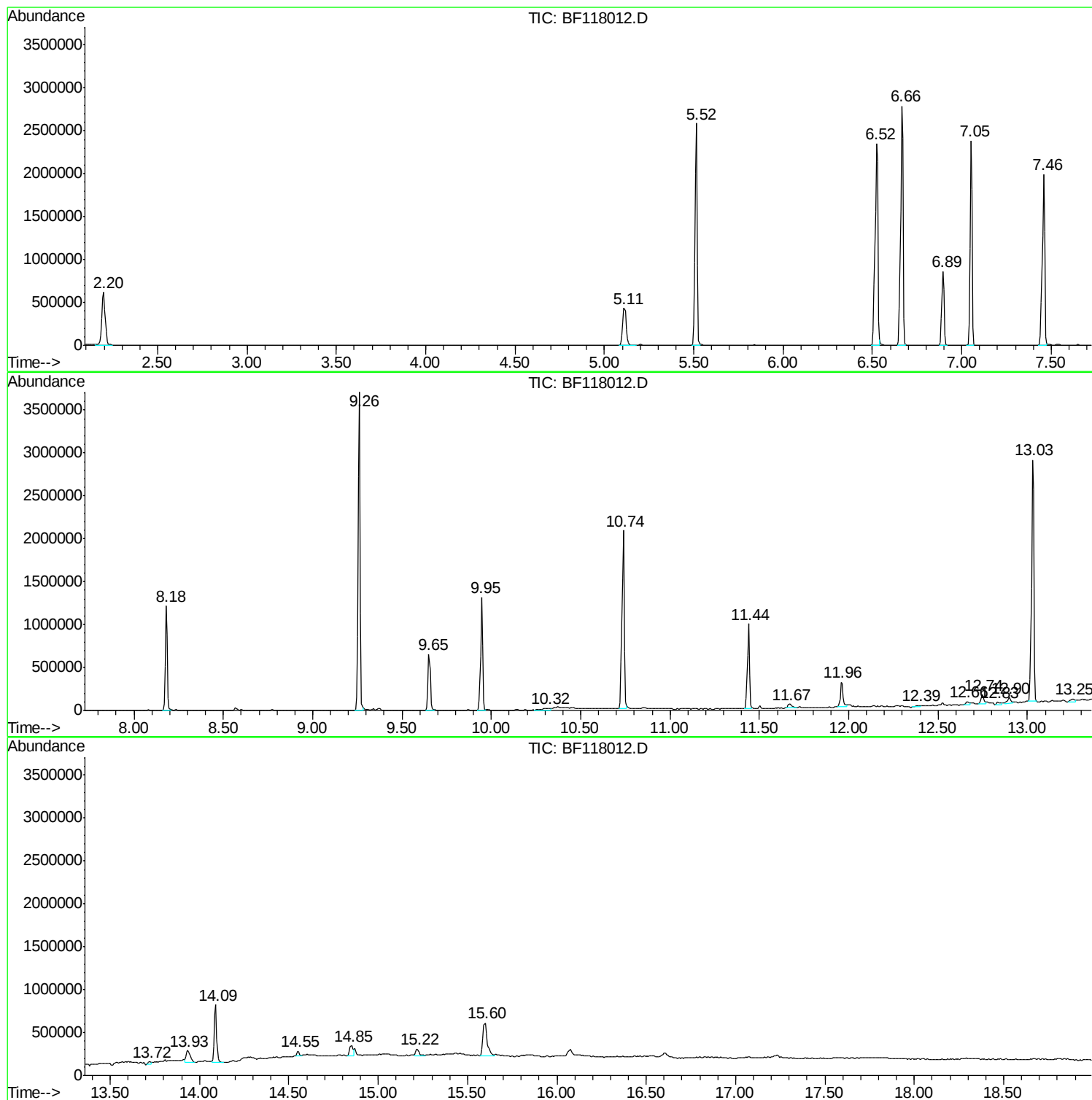
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
B-1-6-12

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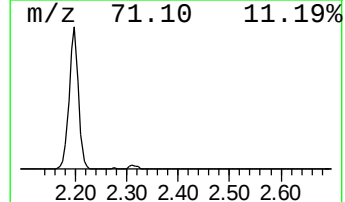
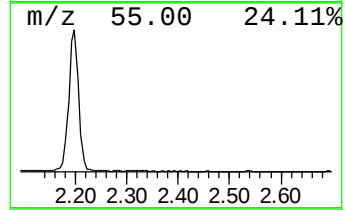
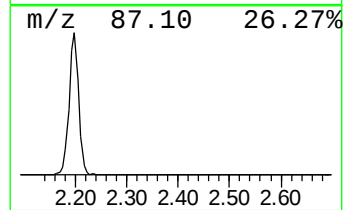
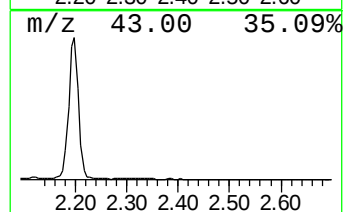
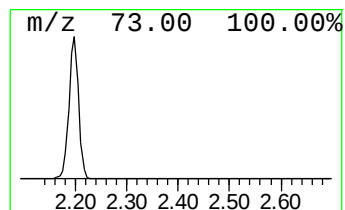
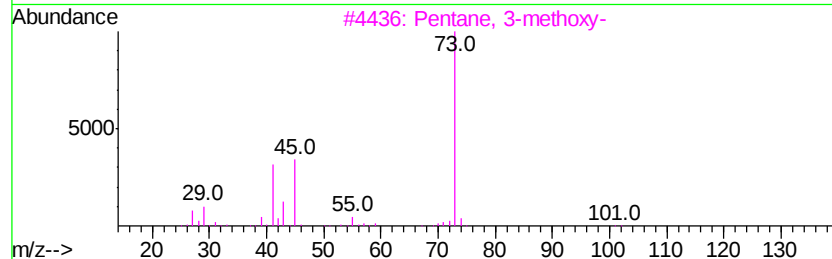
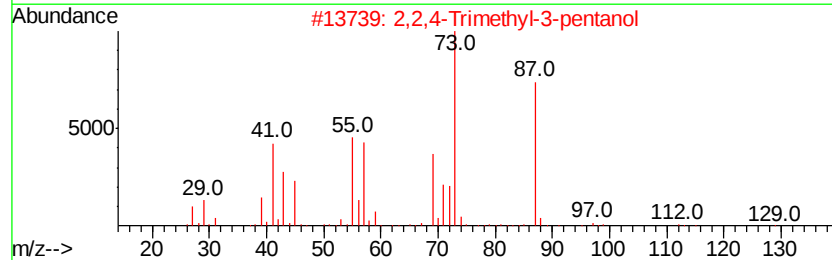
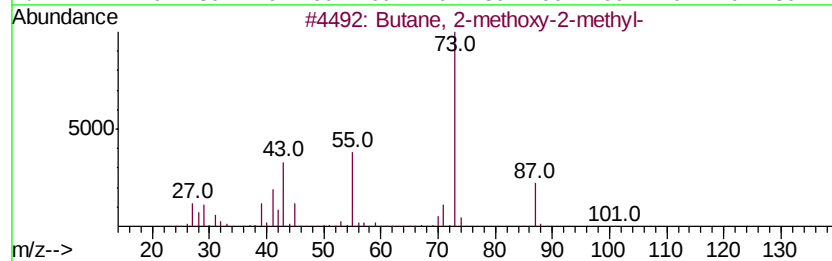
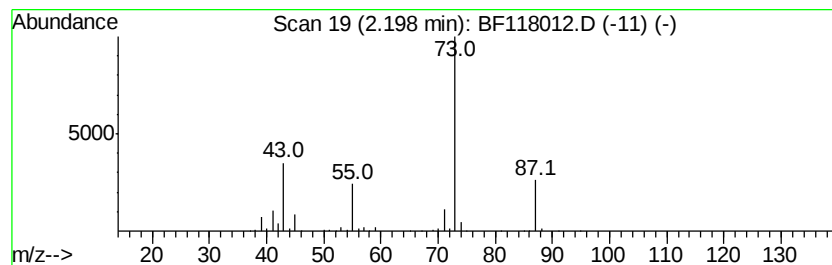
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.20	22.78 ng	801147	1,4-Dichlorobenzene-d4	6.89
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Butane, 2-methoxy-2-methyl-	102 C6H14O	000994-05-8 83
2		2,2,4-Trimethyl-3-pentanol	130 C8H18O	005162-48-1 39
3		Pentane, 3-methoxy-	102 C6H14O	036839-67-5 23
4		1,3-Dioxolane, 2-methyl-	88 C4H8O2	000497-26-7 9
5		Borane, dimethoxy-	74 C2H7BO2	004542-61-4 9



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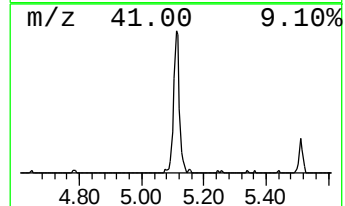
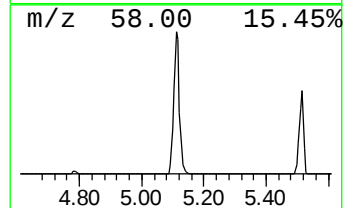
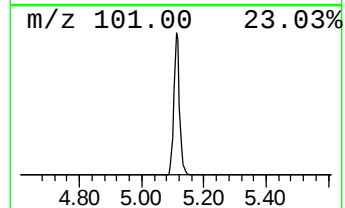
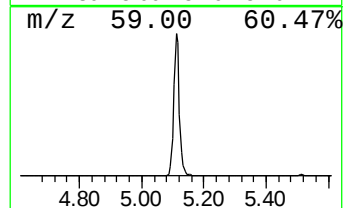
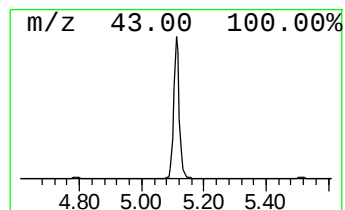
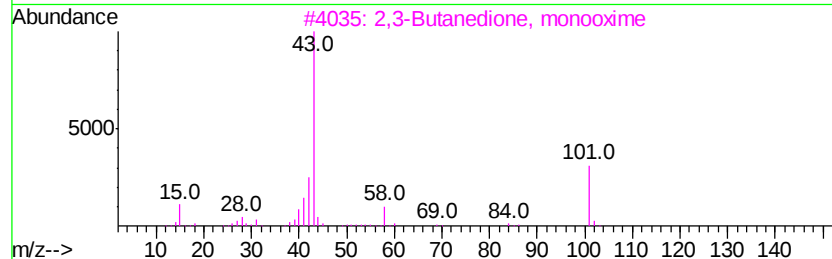
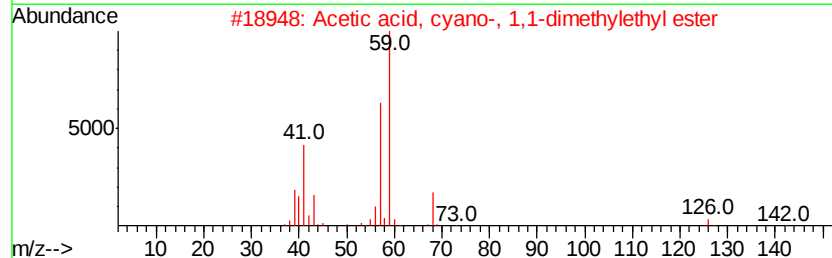
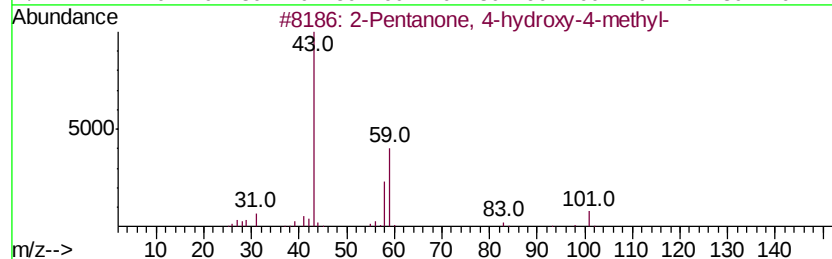
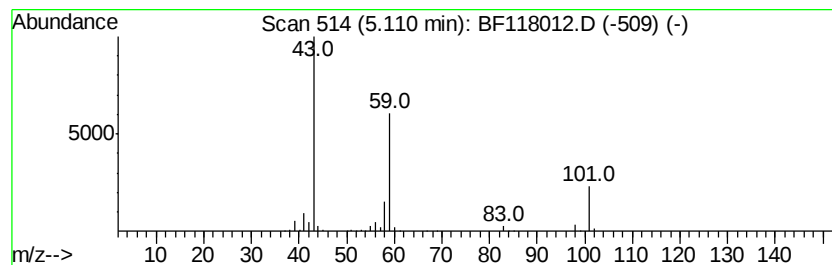
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	15.70 ng	552187	1,4-Dichlorobenzene-d4	6.89

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	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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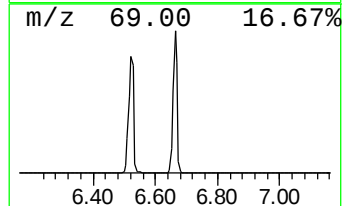
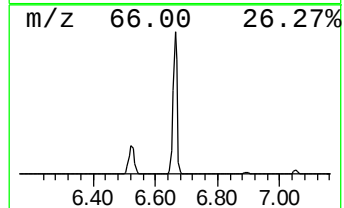
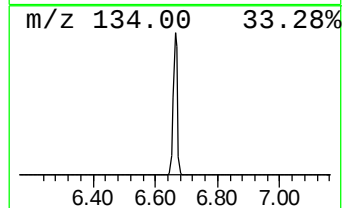
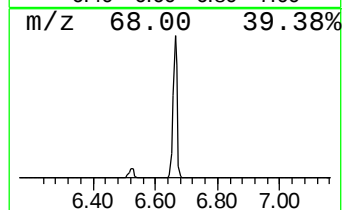
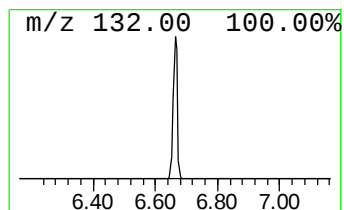
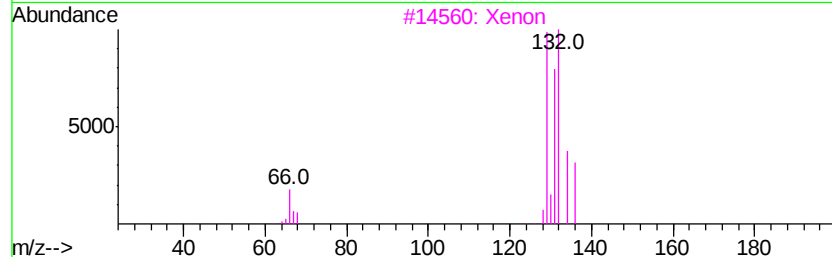
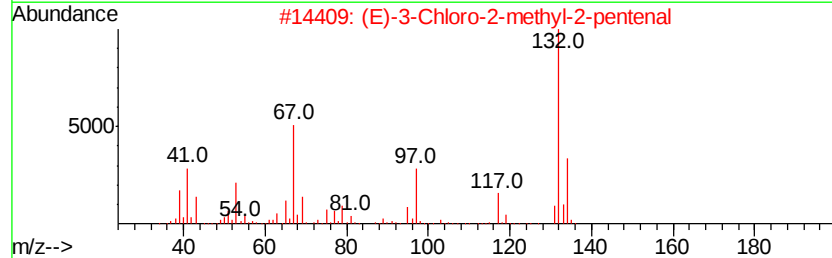
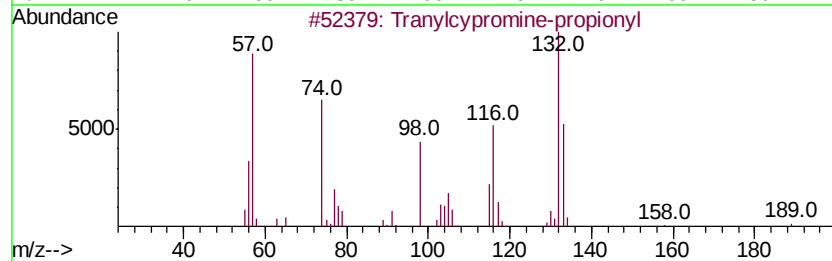
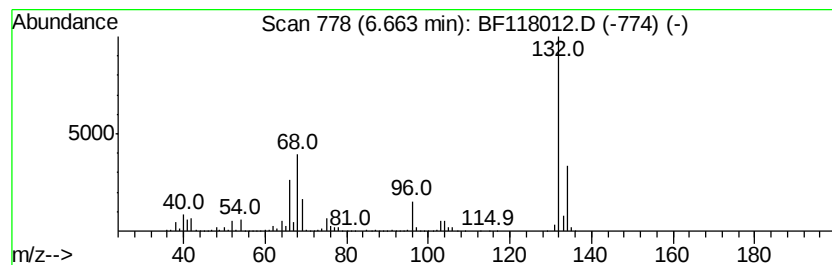
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	76.07 ng	2674940	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		Xenon	132	Xe	007440-63-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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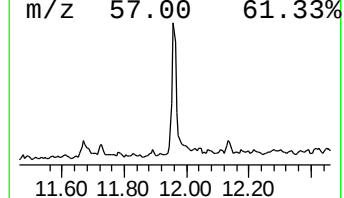
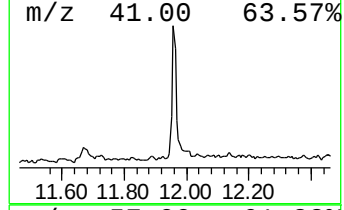
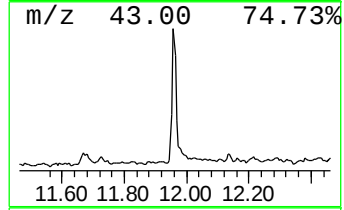
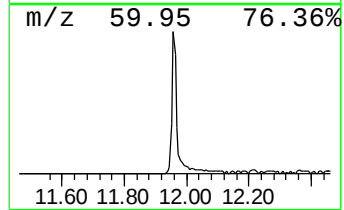
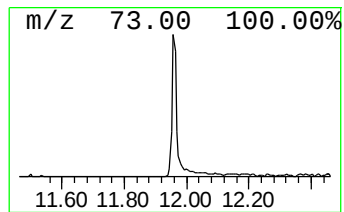
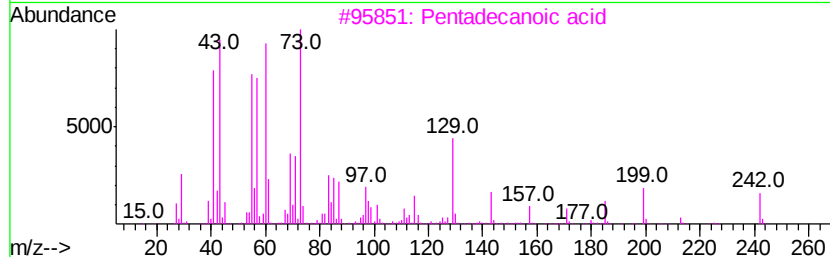
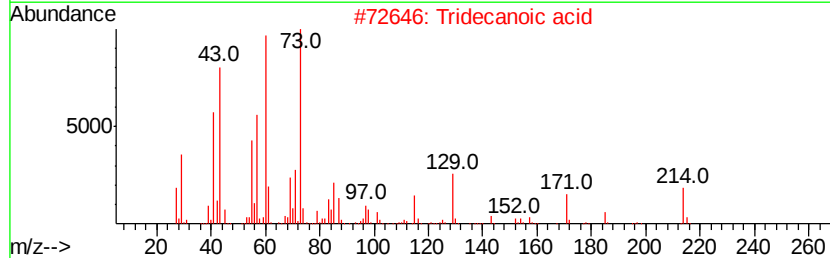
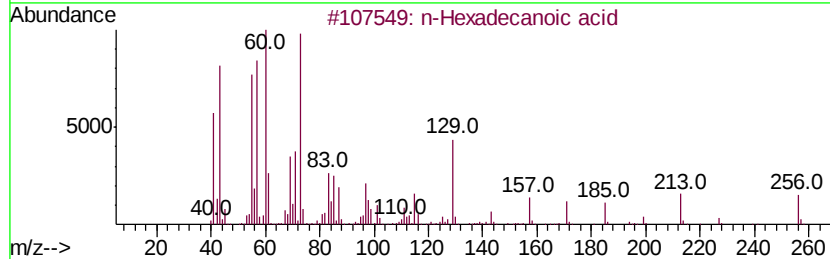
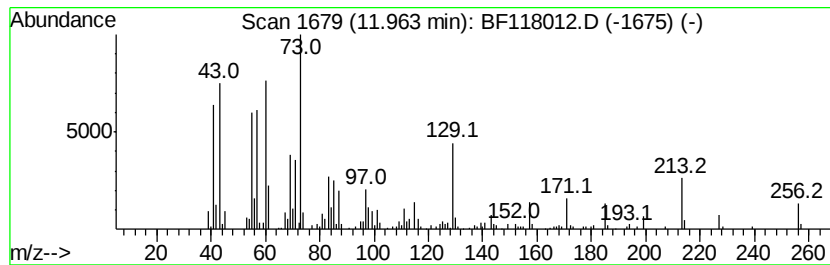
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	7.96 ng	310538	Phenanthrene-d10	11.44

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	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



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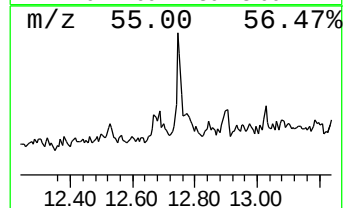
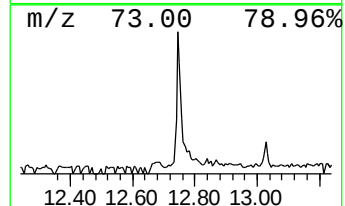
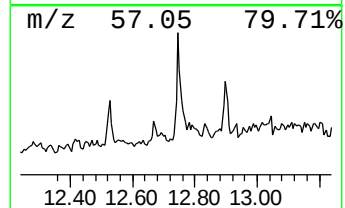
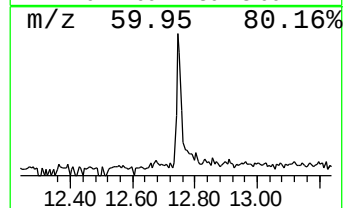
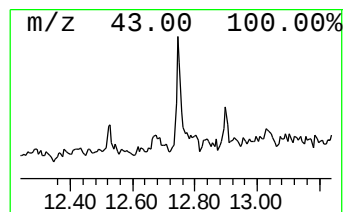
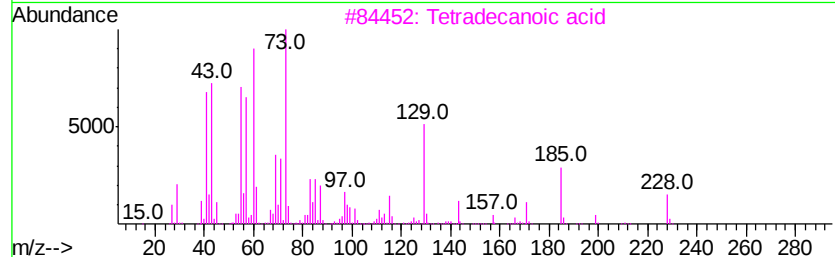
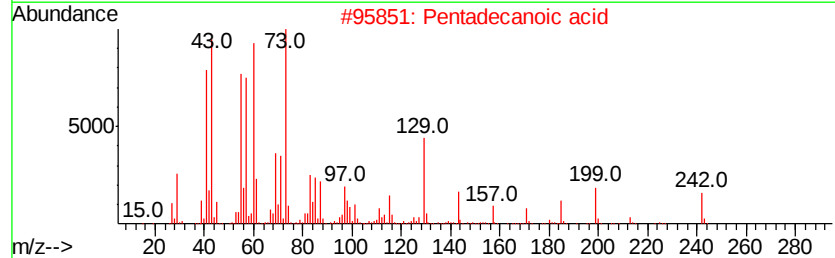
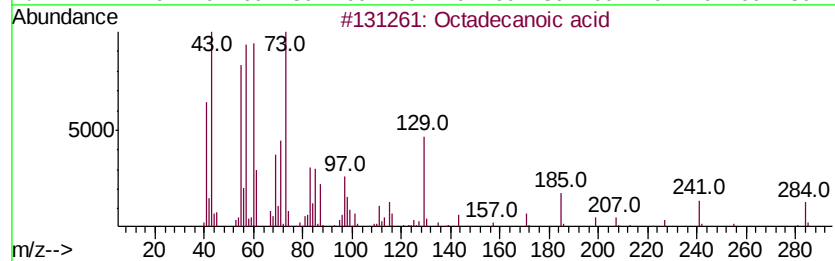
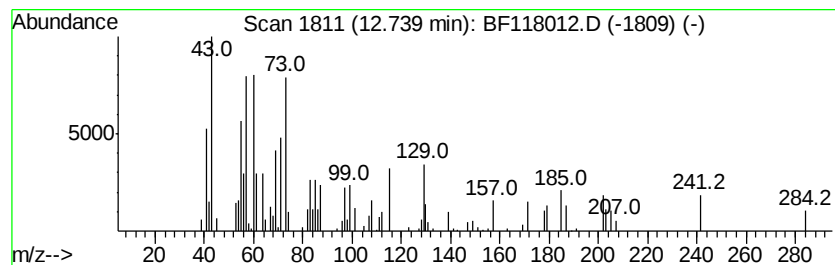
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Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	2.77 ng	108278	Phenanthrene-d10	11.44

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	93
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



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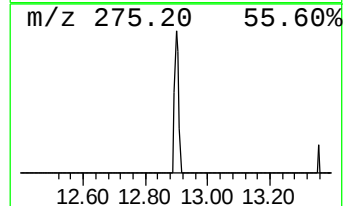
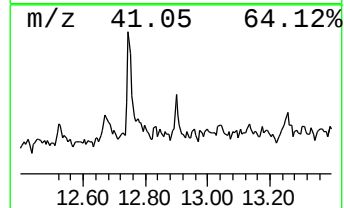
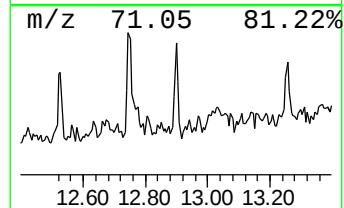
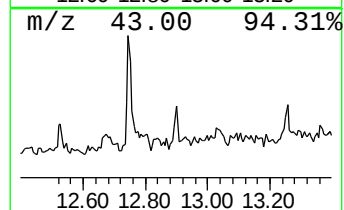
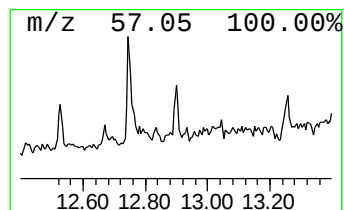
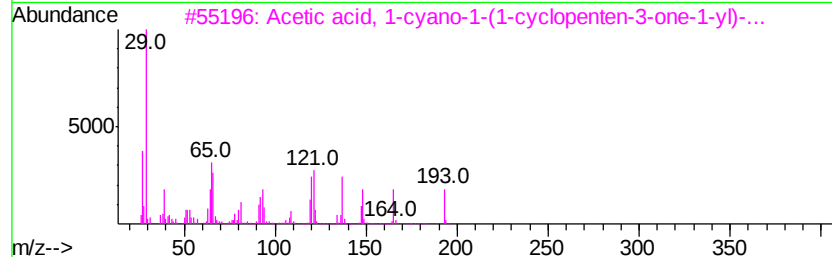
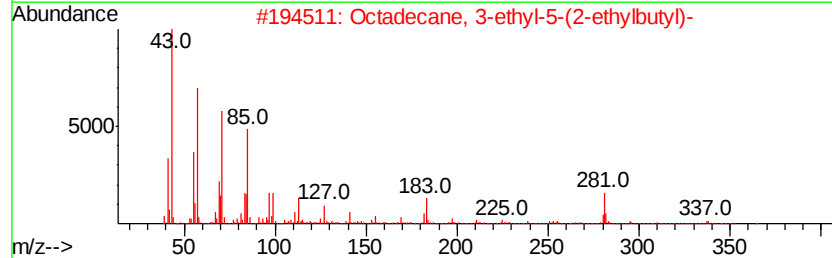
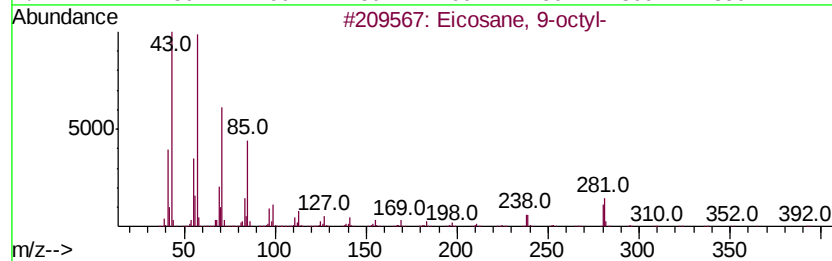
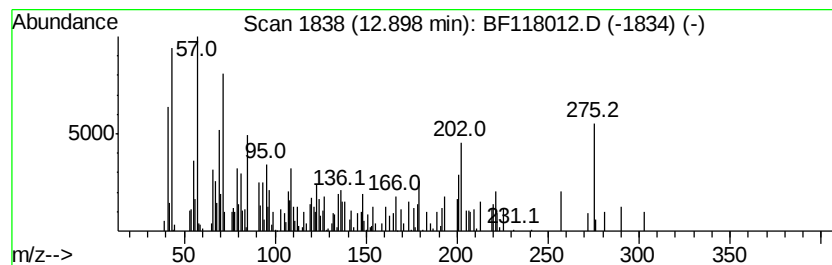
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown12.90 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.90	2.44 ng	75948	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	12
2		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	12
3		Acetic acid, 1-cyano-1-(1-cyclop...	193	C10H11NO3	1000156-29-2	11
4		1,2,5-Triazole, 1-(3-propenyl)-3...	213	C6H7N5O4	311314-76-8	10
5		Dioctyl disulphide	290	C16H34S2	000822-27-5	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118012.D
Acq On : 26 Nov 2019 17:32
Operator : JU
Sample : K5948-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-1-6-12

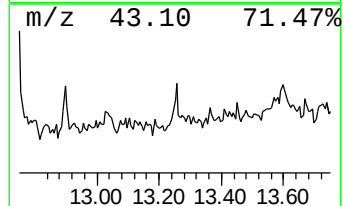
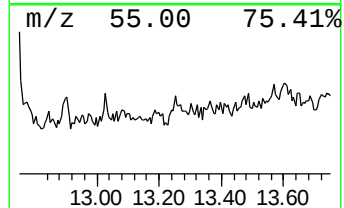
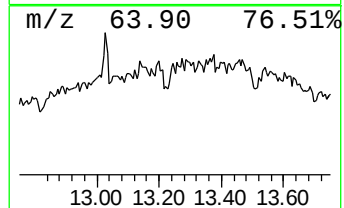
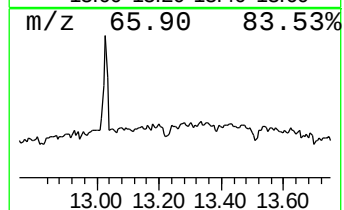
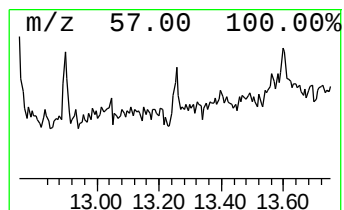
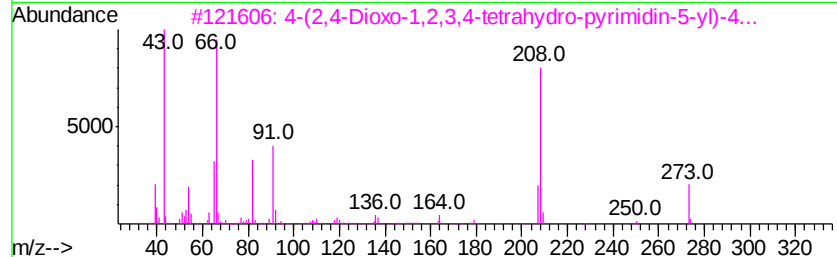
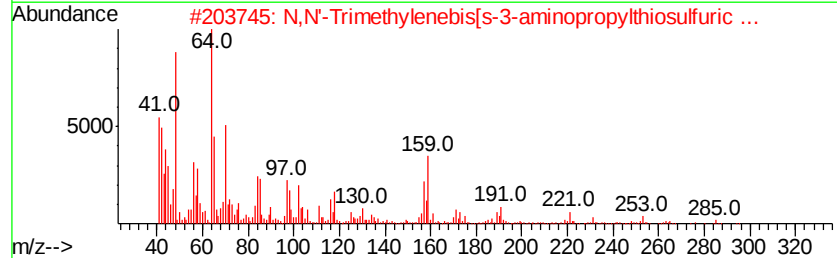
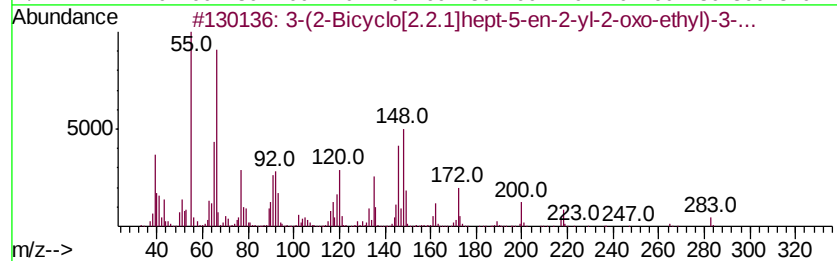
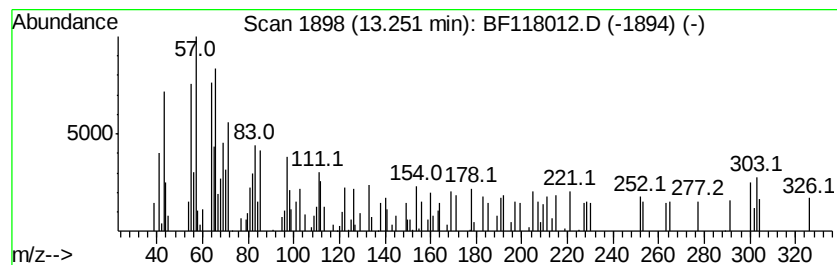
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown13.25 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	2.16 ng	67128	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3	(2-Bicyclo[2.2.1]hept-5-en-2-v...	283	C17H17N03	1000300-35-9	32
2	N,N'	Trimethylenebis[s-3-aminopr...	382	C9H22N2O6S4	035871-60-4	25
3	4	(2,4-Dioxo-1,2,3,4-tetrahydro-...	273	C13H11N3O4	1000300-05-4	22
4	4,7	Methano-1H-indene, 2,3,3a,4,...	134	C10H14	019398-83-5	22
5	4,7	Methanoindene, 3a,4,5,6,7,7a...	134	C10H14	002825-86-7	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
 Data File : BF118012.D
 Acq On : 26 Nov 2019 17:32
 Operator : JU
 Sample : K5948-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-1-6-12

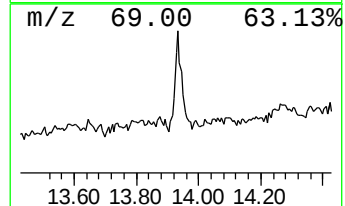
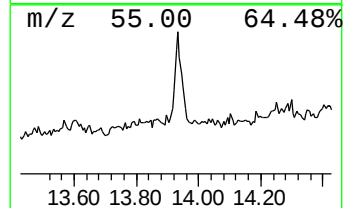
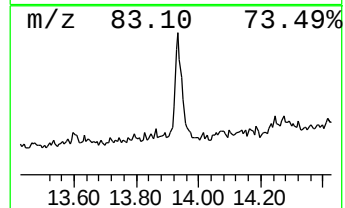
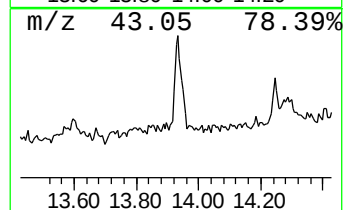
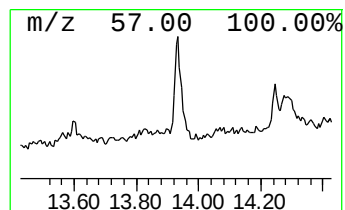
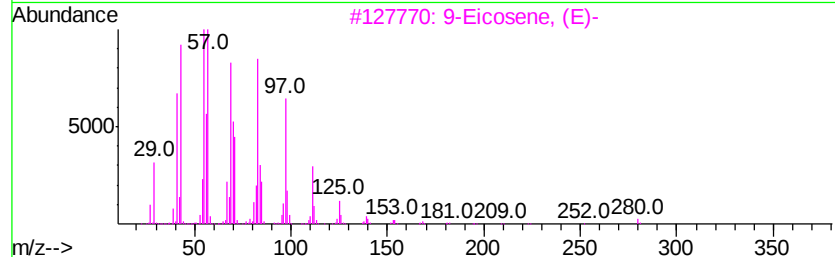
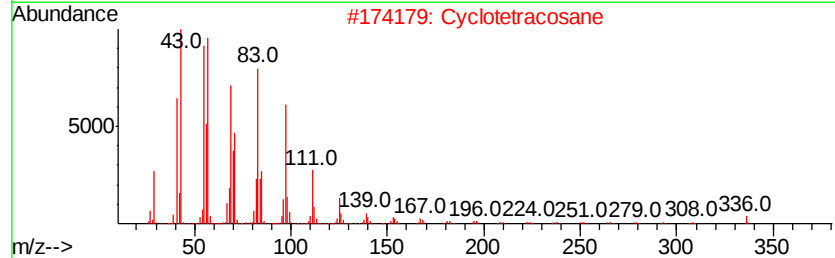
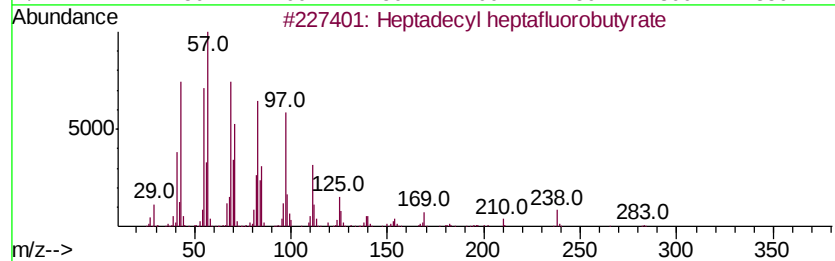
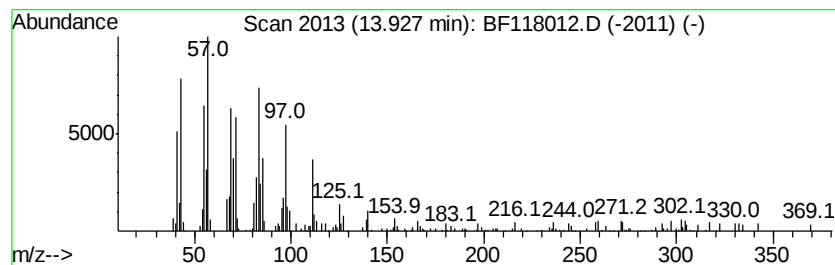
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.53 ng	234208	Chrysene-d12	14.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	94
2			Cyclotetracosane	336	C24H48	000297-03-0	93
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118012.D
Acq On : 26 Nov 2019 17:32
Operator : JU
Sample : K5948-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-1-6-12

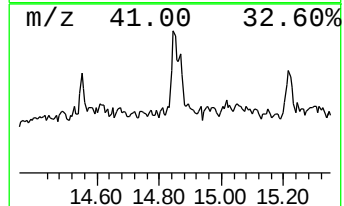
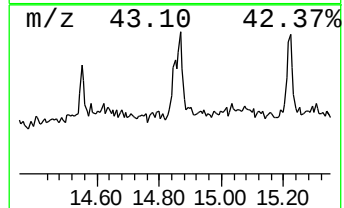
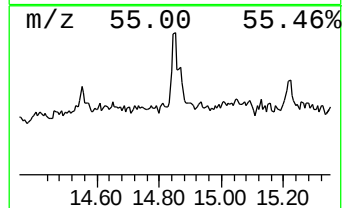
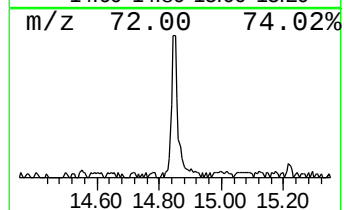
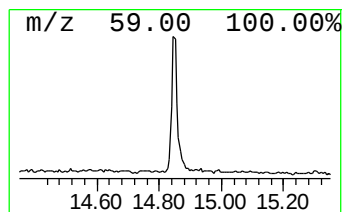
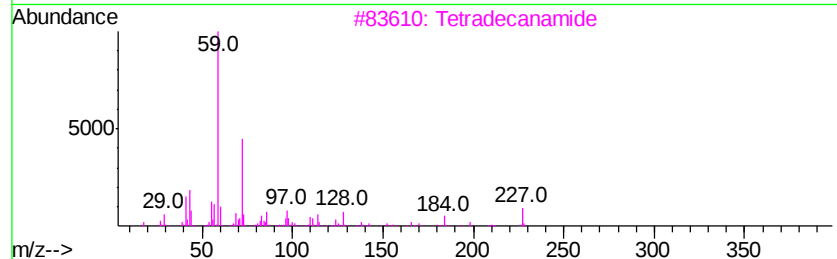
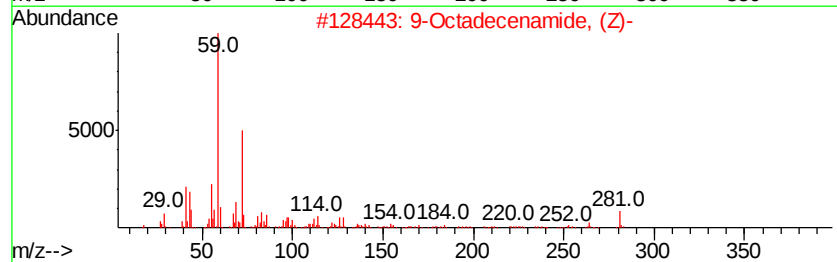
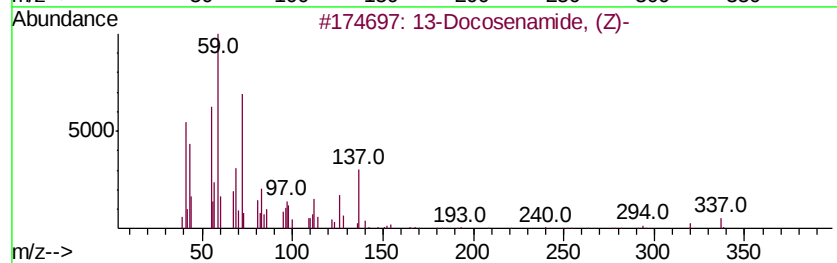
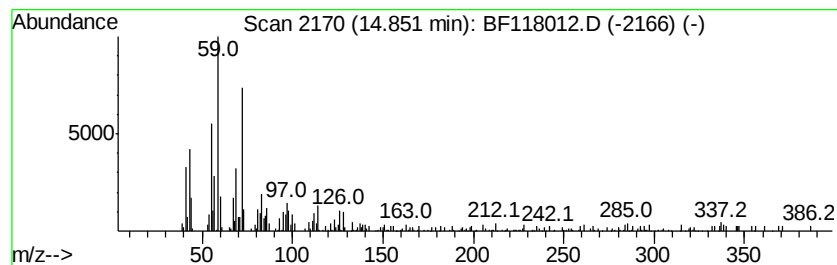
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 13-Docosenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	5.23 ng	157915	Perylene-d12	15.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	93
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
3		Tetradecanamide	227	C14H29NO	000638-58-4	50
4		Octadecanamide	283	C18H37NO	000124-26-5	43
5		Dodecanamide	199	C12H25NO	001120-16-7	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112619\
Data File : BF118012.D
Acq On : 26 Nov 2019 17:32
Operator : JU
Sample : K5948-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
B-1-6-12

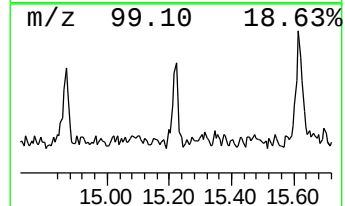
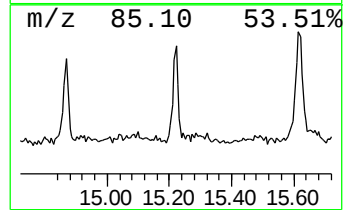
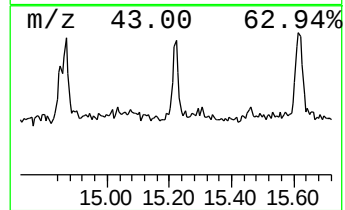
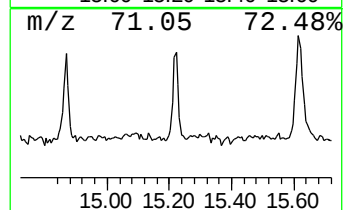
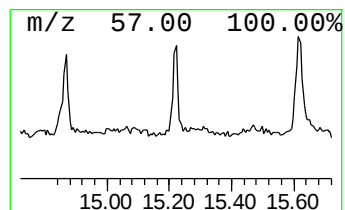
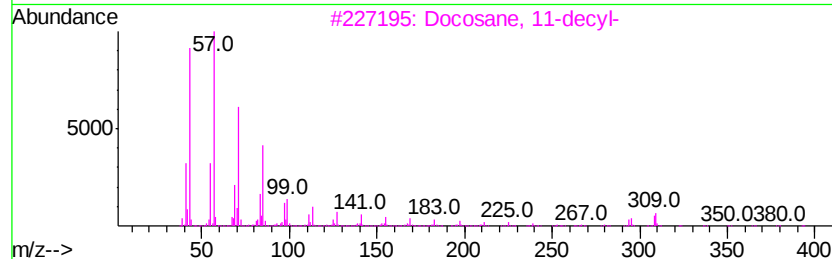
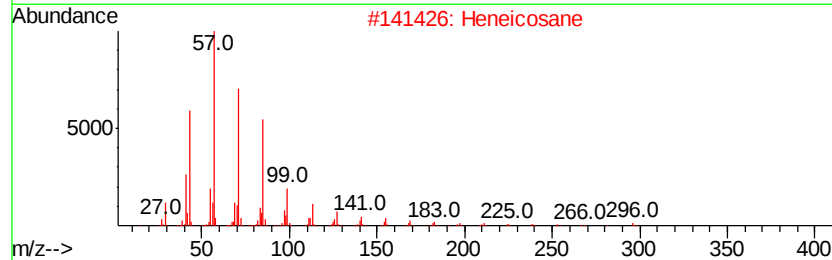
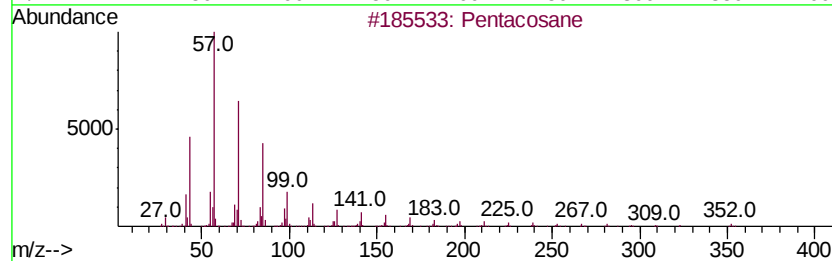
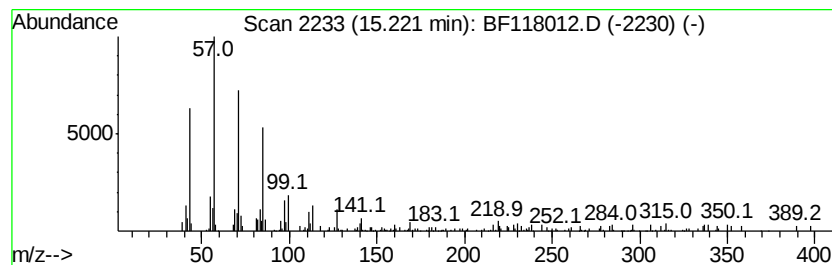
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.93 ng	88451	Perylene-d12	15.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentacosane	352	C25H52	000629-99-2	97
2		Heneicosane	296	C21H44	000629-94-7	93
3		Docosane, 11-decyl-	451	C32H66	055401-55-3	86
4		2-methyloctacosane	408	C29H60	1000376-72-8	86
5		Hexacosane	366	C26H54	000630-01-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112619\
 Data File : BF118012.D
 Acq On : 26 Nov 2019 17:32
 Operator : JU
 Sample : K5948-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-1-6-12

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
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2-Pentanone, 4-hy...	5.11	15.7	ng	552187	1	6.89	703297	20.0
unknown6.66	6.66	76.1	ng	2674940	1	6.89	703297	20.0
n-Hexadecanoic acid	11.96	8.0	ng	310538	4	11.44	780477	20.0
Octadecanoic acid	12.74	2.8	ng	108278	4	11.44	780477	20.0
unknown12.90	12.90	2.4	ng	75948	5	14.09	622469	20.0
unknown13.25	13.25	2.2	ng	67128	5	14.09	622469	20.0
Heptadecyl heptaf...	13.93	7.5	ng	234208	5	14.09	622469	20.0
13-Docosenamide, ...	14.85	5.2	ng	157915	6	15.60	603660	20.0
Pentacosane	15.22	2.9	ng	88451	6	15.60	603660	20.0