

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
 Data File : BF118833.D
 Acq On : 6 Feb 2020 12:22
 Operator : CG/JU
 Sample : PB126588BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB126588BL

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-BF020320.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	2.898	132	138	148	rVB	76899	135779	1.38%	0.234%
2	5.434	565	569	572	rBV	2925683	2655318	27.04%	4.574%
3	6.439	736	740	753	rBV	1863751	1707979	17.39%	2.942%
4	6.810	800	803	807	rBV	1645819	1465608	14.92%	2.525%
5	6.969	826	830	834	rBV	5184635	5122550	52.16%	8.825%
6	7.375	893	899	902	rBV	4132009	4269718	43.48%	7.355%
7	8.092	1016	1021	1025	rBV	2041277	1806829	18.40%	3.113%
8	8.480	1083	1087	1093	rBV	99426	112678	1.15%	0.194%
9	9.175	1199	1205	1208	rBV	7274854	7851325	79.94%	13.525%
10	9.292	1219	1225	1240	rVB	579957	658379	6.70%	1.134%
11	9.563	1267	1271	1281	rVB	447718	407180	4.15%	0.701%
12	9.845	1314	1319	1331	rBV	2363119	2454940	25.00%	4.229%
13	10.633	1448	1453	1467	rBV	4418593	4540815	46.24%	7.822%
14	11.327	1567	1571	1575	rBV	2655203	2615485	26.63%	4.506%
15	11.569	1607	1612	1619	rBV4	68320	117311	1.19%	0.202%
16	11.786	1645	1649	1654	rBV	185870	200889	2.05%	0.346%
17	11.868	1657	1663	1677	rVV	1529663	1786925	18.20%	3.078%
18	12.568	1776	1782	1791	rBV4	127988	253597	2.58%	0.437%
19	12.645	1792	1795	1808	rVV	626697	708856	7.22%	1.221%
20	12.921	1836	1842	1845	rBV	9252632	9820963	100.00%	16.919%
21	13.821	1989	1995	2008	rBV2	474708	727669	7.41%	1.254%
22	13.968	2014	2020	2027	rBV	2311654	2326722	23.69%	4.008%
23	14.139	2045	2049	2053	rBV	251730	242552	2.47%	0.418%
24	14.439	2096	2100	2112	rBV	448016	445013	4.53%	0.767%
25	14.745	2148	2152	2156	rVB	512794	525166	5.35%	0.905%
26	14.815	2160	2164	2169	rBV	1021807	1014088	10.33%	1.747%
27	15.074	2203	2208	2213	rBV	560571	616161	6.27%	1.061%
28	15.409	2260	2265	2269	rBV	1374382	1931264	19.66%	3.327%
29	15.445	2269	2271	2283	rVB	562242	647406	6.59%	1.115%
30	15.868	2338	2343	2349	rBV	327304	473574	4.82%	0.816%
31	16.362	2421	2427	2433	rVB	160898	286098	2.91%	0.493%
32	16.939	2519	2525	2534	rVB	56551	119492	1.22%	0.206%

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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF020320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

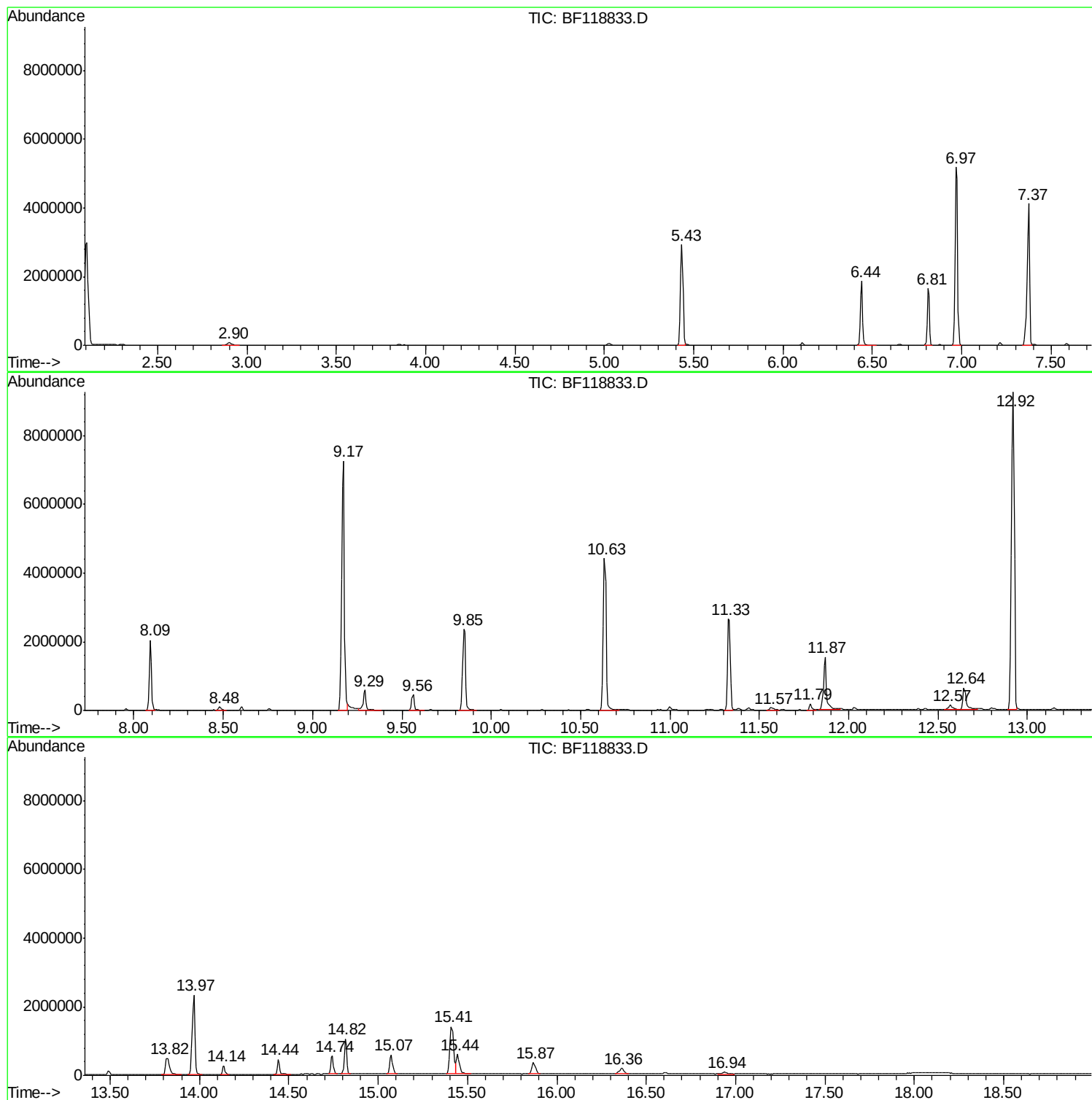
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Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF020320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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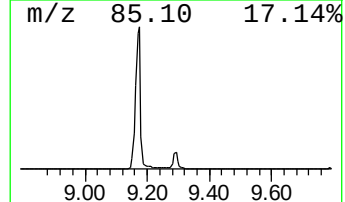
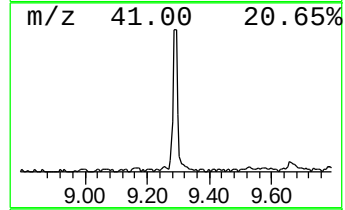
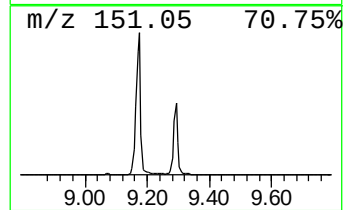
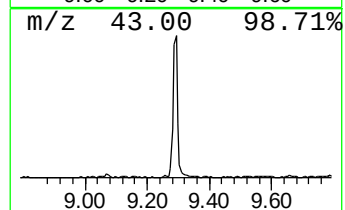
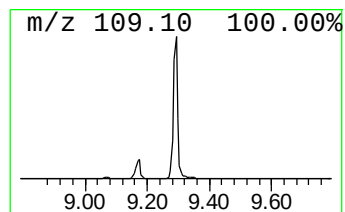
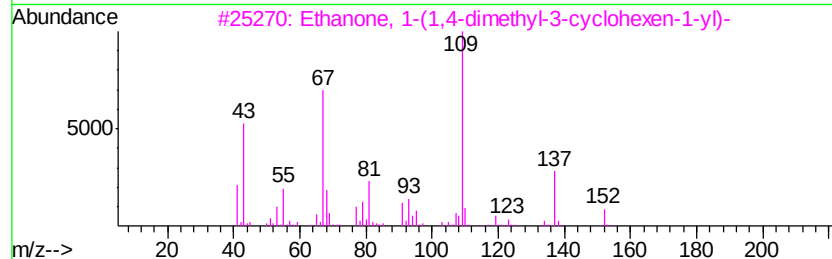
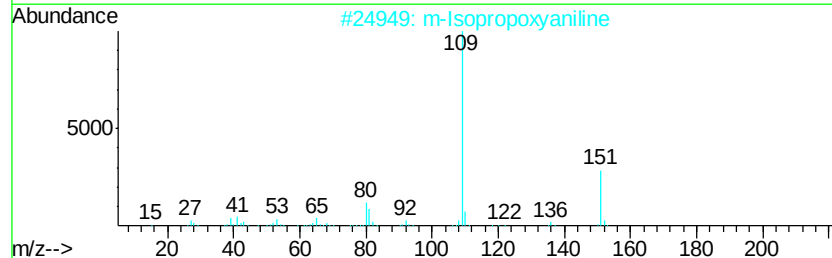
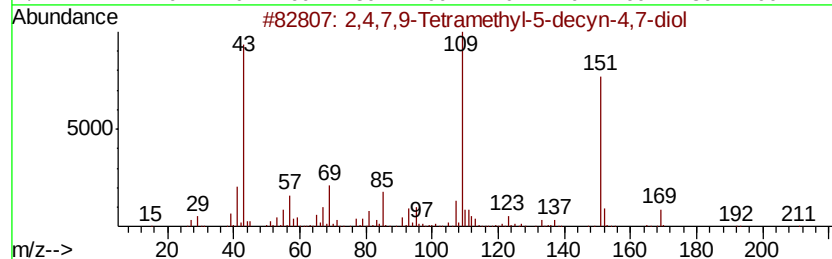
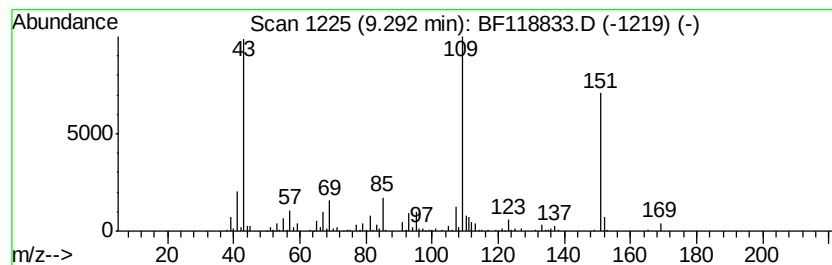
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	5.36 ng	658379	Acenaphthene-d10	9.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2			m-Isopropoxyaniline	151	C9H13NO	041406-00-2	53
3			Ethanone, 1-(1,4-dimethyl-3-cyclo...	152	C10H16O	043219-68-7	47
4			(7,7-Dimethyl-2-oxobicyclo[2.2.1...	250	C10H15ClO3S	1000194-76-1	42
5			N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	38



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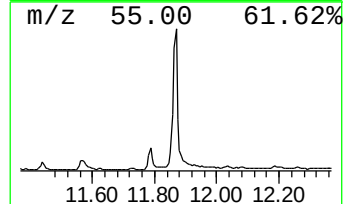
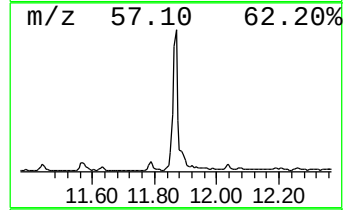
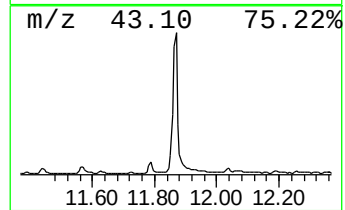
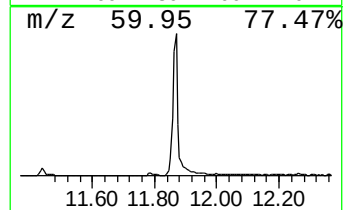
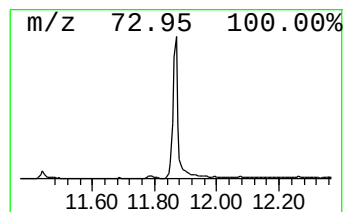
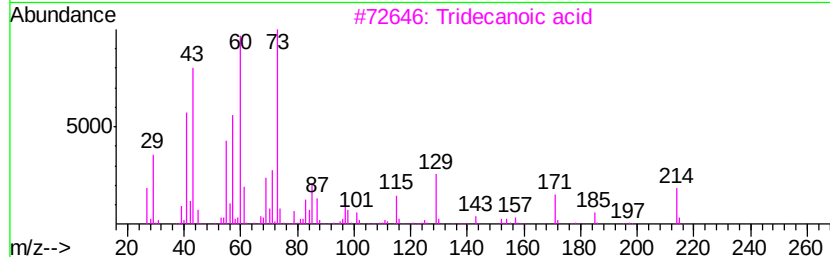
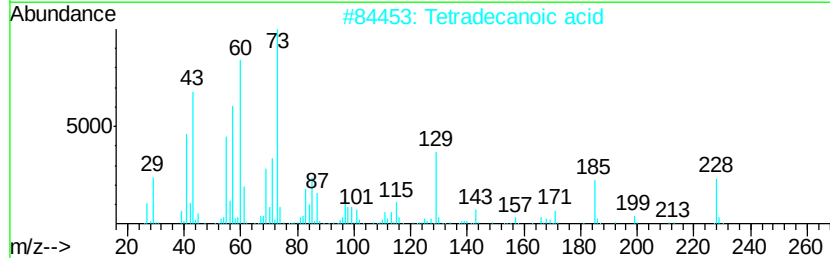
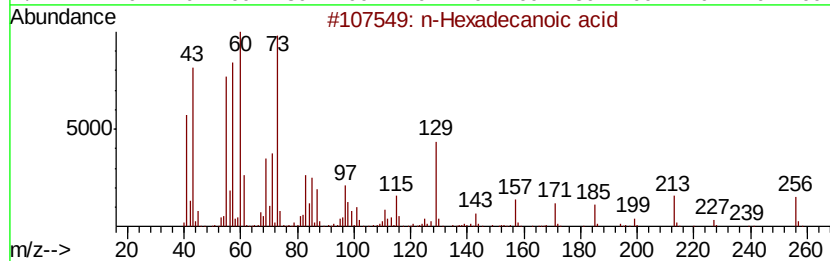
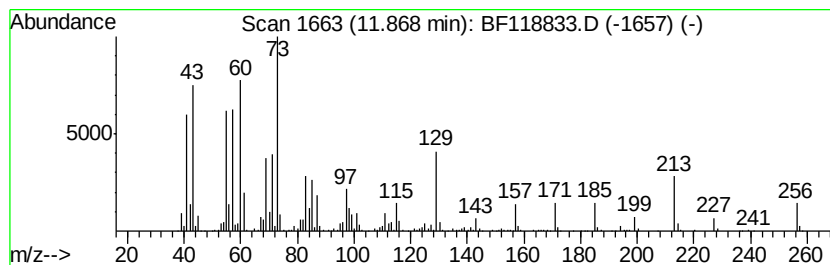
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	13.66 ng	1786930	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	89
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



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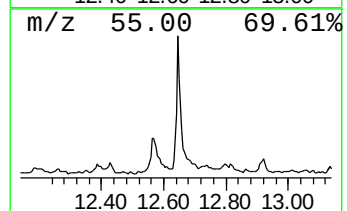
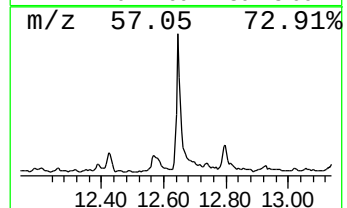
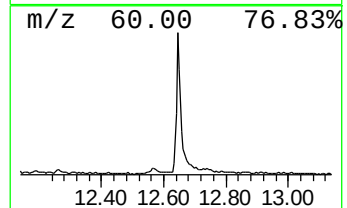
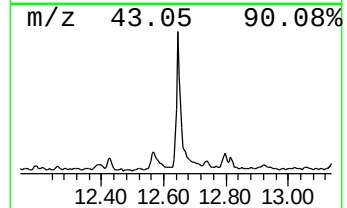
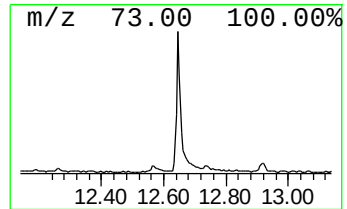
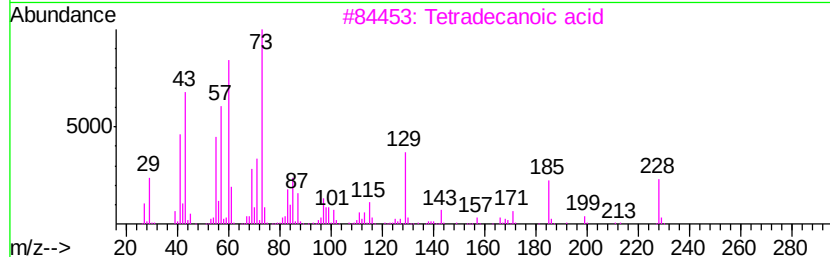
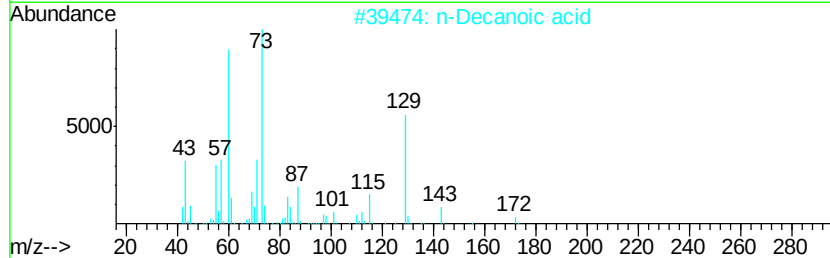
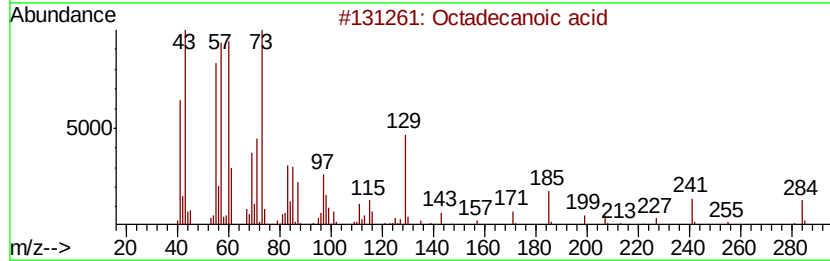
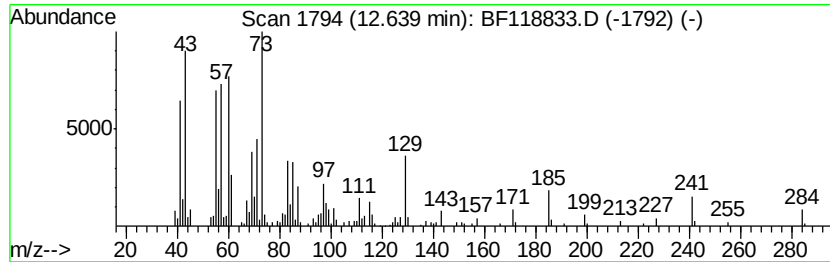
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	5.42 ng	708856	Phenanthrene-d10	11.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5		Tridecanoic acid	214	C13H26O2	000638-53-9	76



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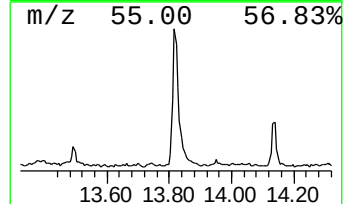
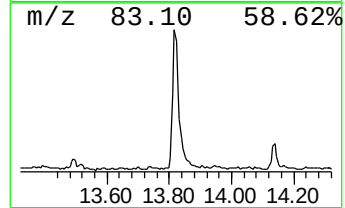
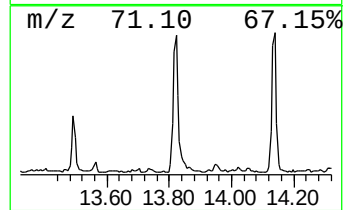
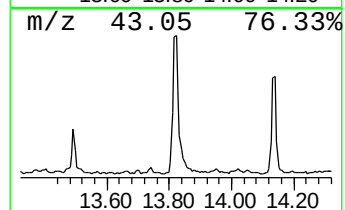
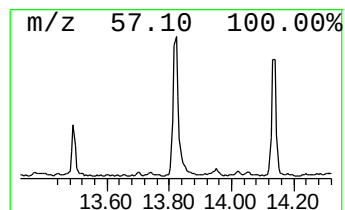
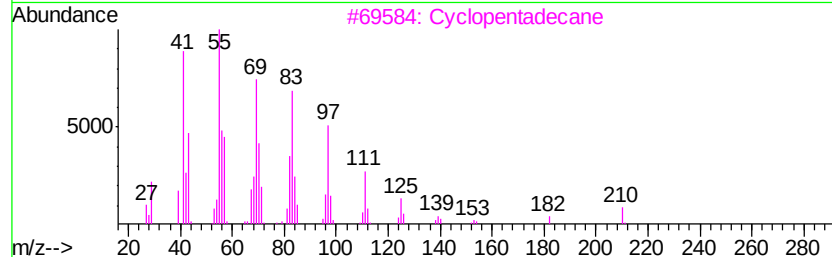
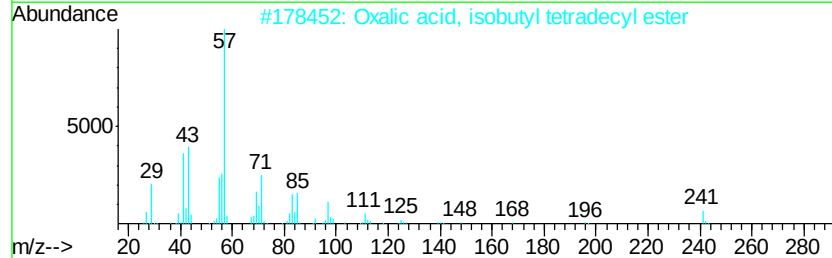
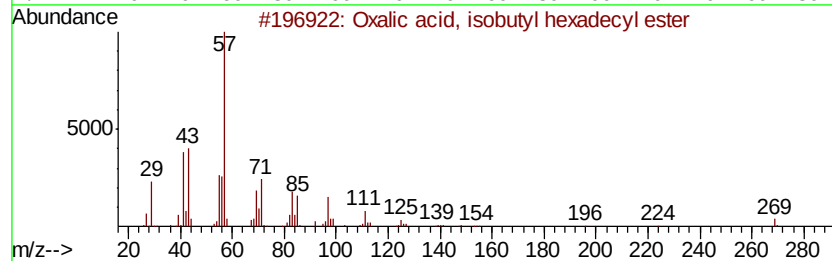
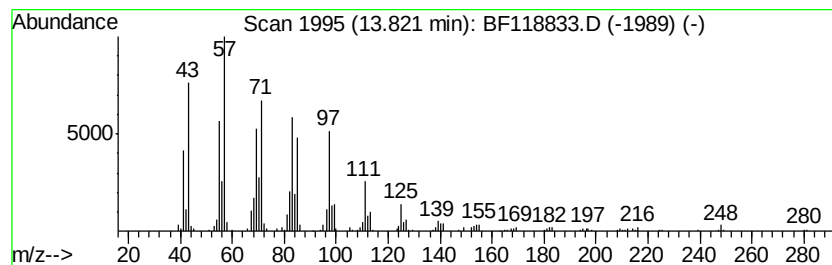
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Oxalic acid, isobutyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	6.25 ng	727669	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2		Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	91
3		Cyclopentadecane	210	C15H30	000295-48-7	90
4		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87



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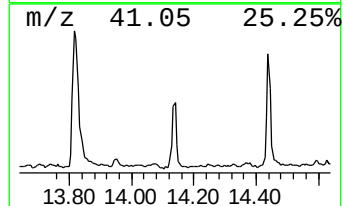
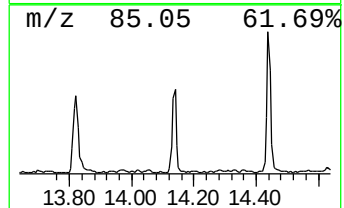
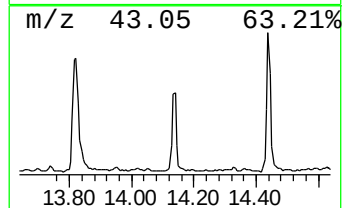
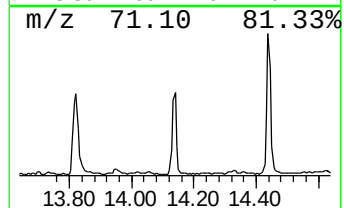
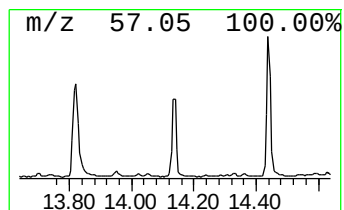
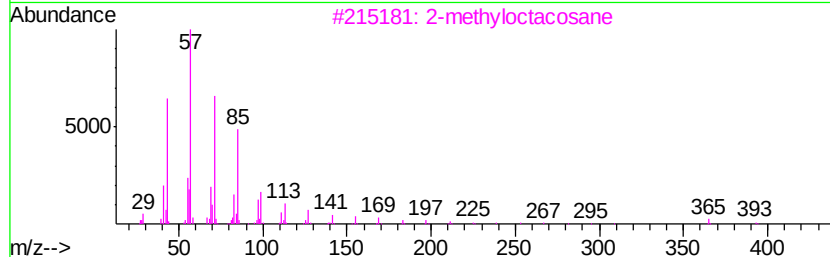
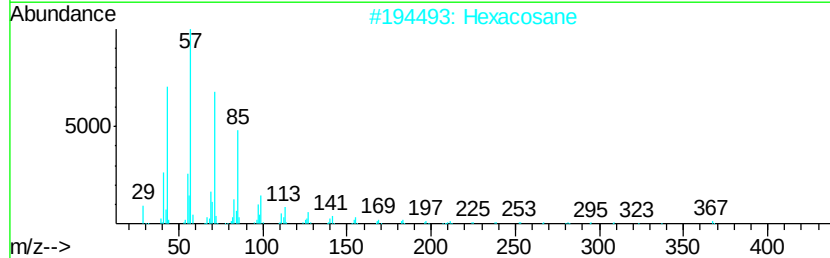
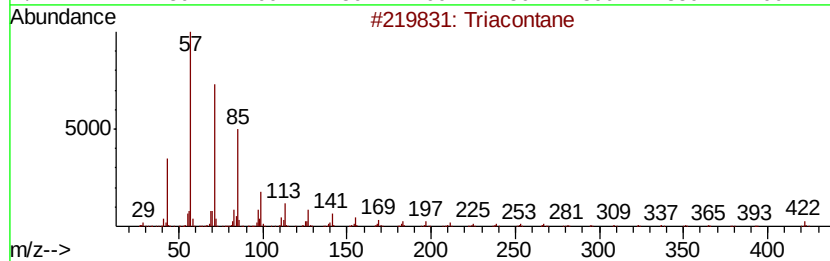
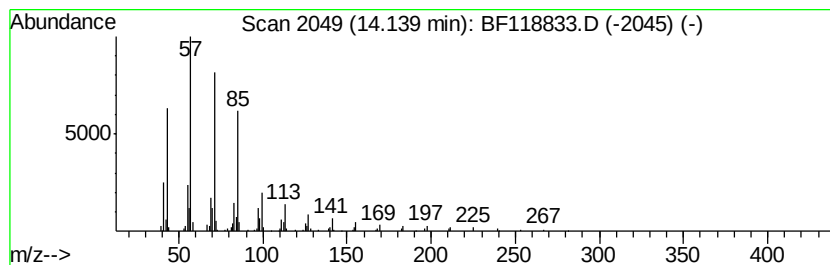
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Triacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.08 ng	242552	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		2-methyloctacosane	408	C29H60	1000376-72-8	91
4		Heneicosane	296	C21H44	000629-94-7	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



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PB126588BL

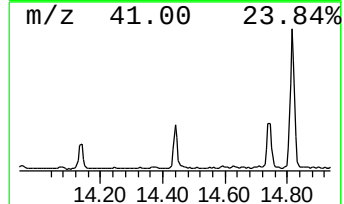
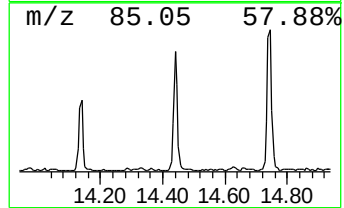
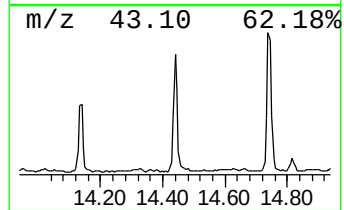
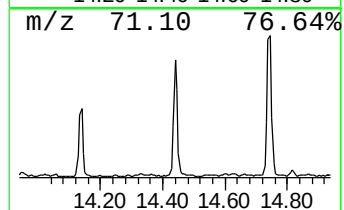
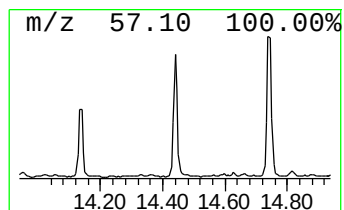
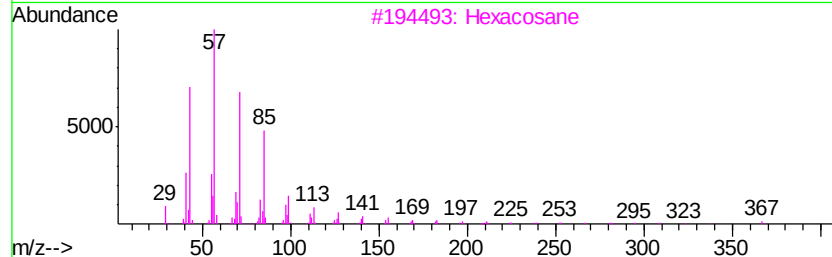
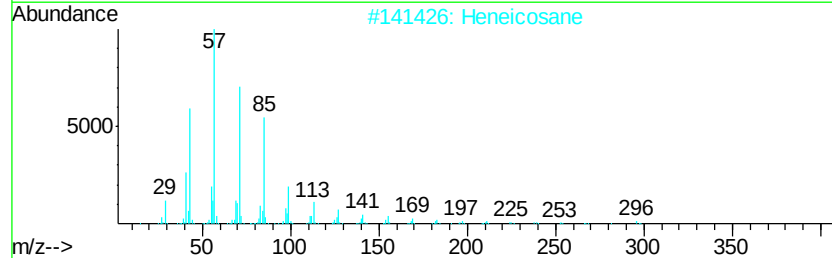
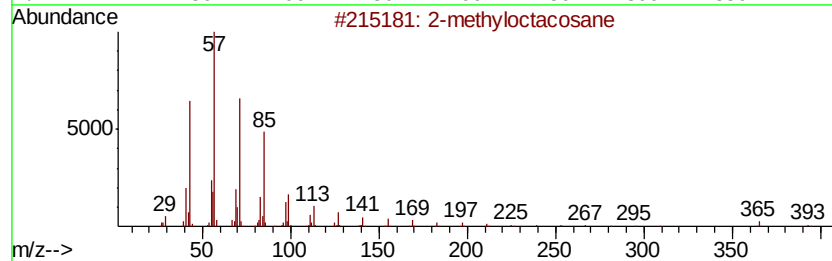
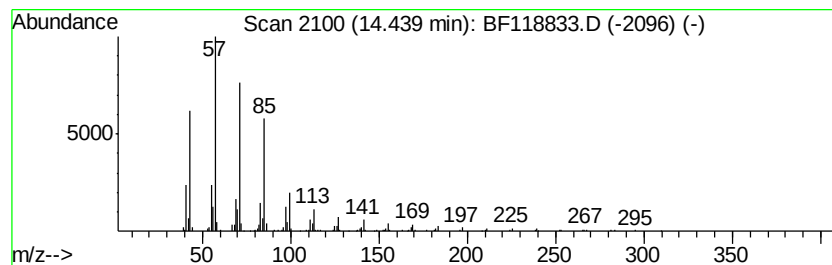
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	3.83 ng	445013	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	90
4		Octacosane	394	C28H58	000630-02-4	90
5		Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
Data File : BF118833.D
Acq On : 6 Feb 2020 12:22
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB126588BL

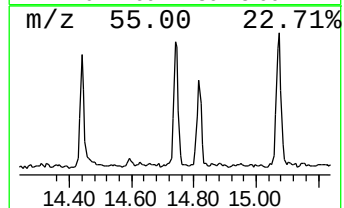
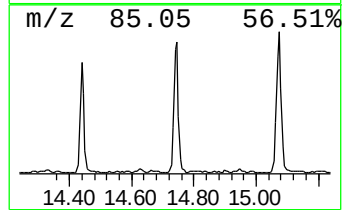
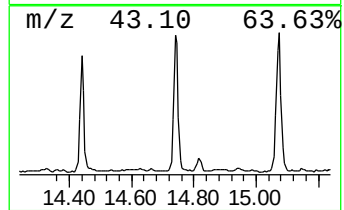
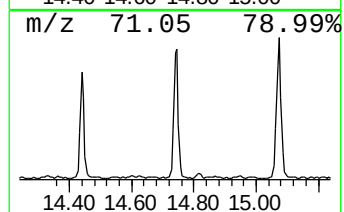
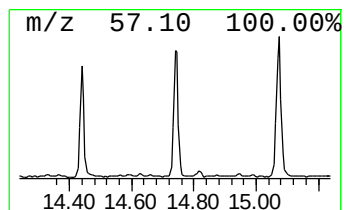
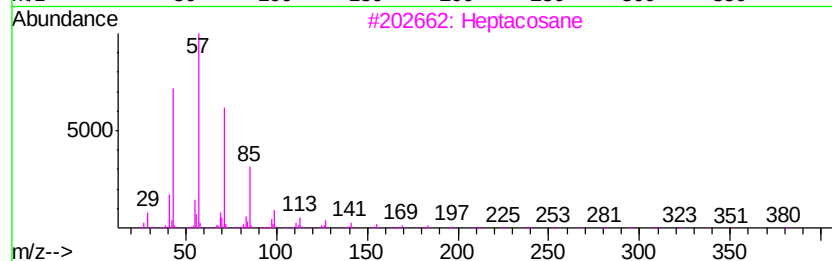
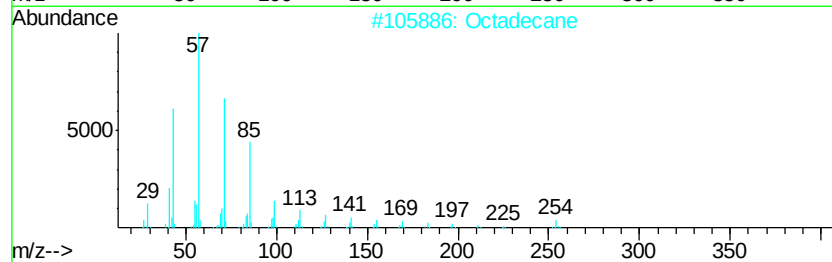
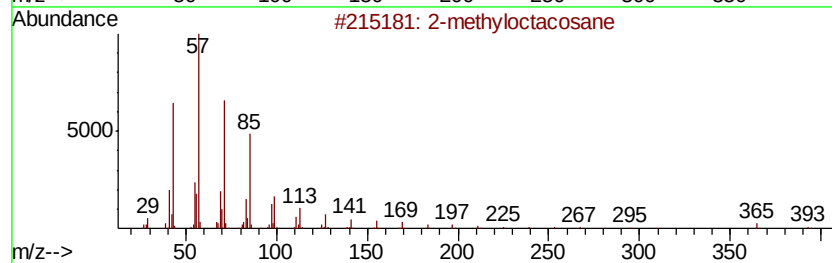
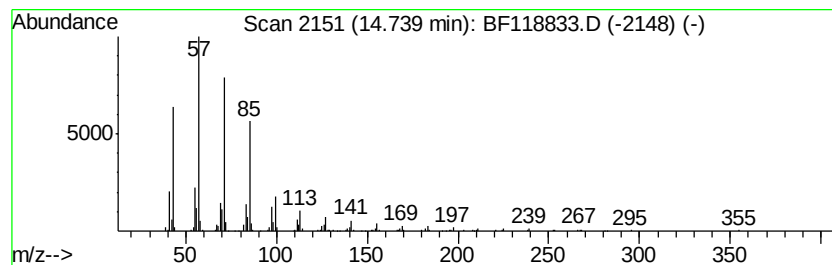
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.74	5.44 ng	525166	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Octadecane	254	C18H38	000593-45-3	91
3		Heptacosane	380	C27H56	000593-49-7	91
4		triacontane	422	C30H62	000638-68-6	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
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Misc :
ALS Vial : 4 Sample Multiplier: 1

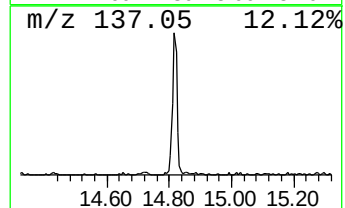
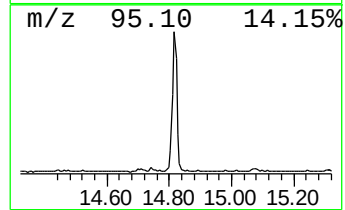
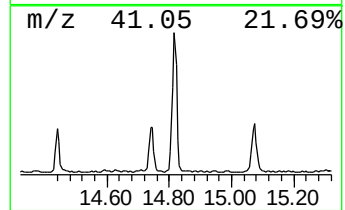
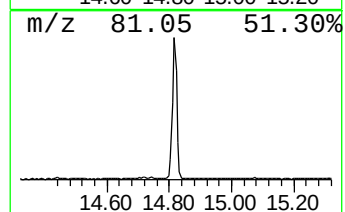
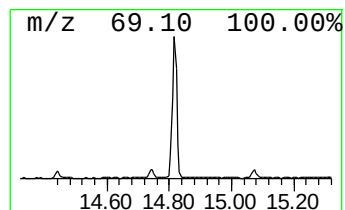
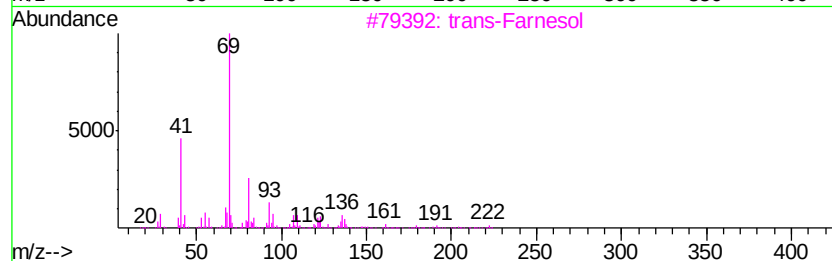
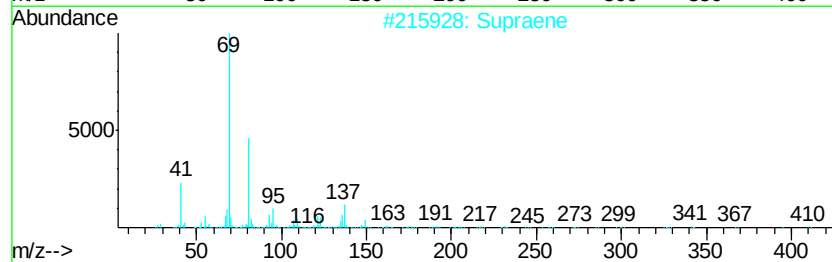
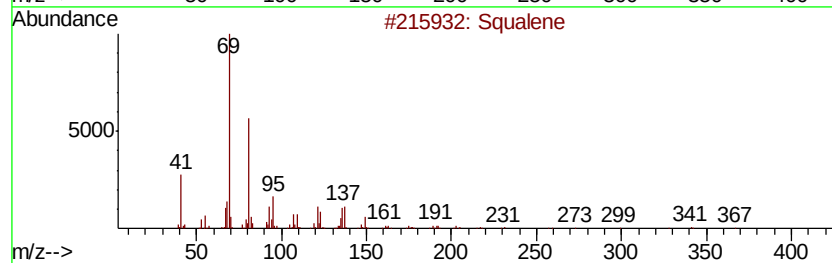
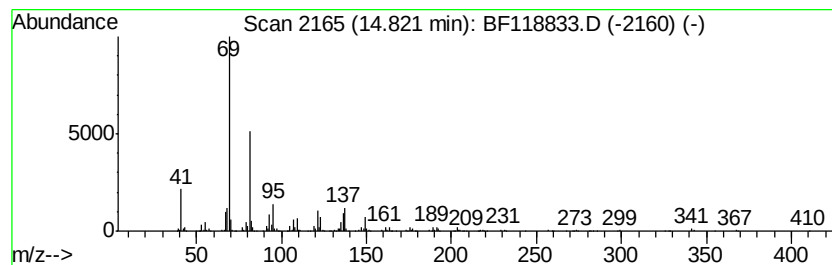
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	10.50 ng	1014090	Perylene-d12	15.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	94
2	Supraene	410 C30H50	007683-64-9	91
3	trans-Farnesol	222 C15H26O	000106-28-5	64
4	4-Methyl-1,5-Heptadiene	110 C8H14	000998-94-7	50
5	2,6-Octadiene, 4-methyl-	124 C9H16	074498-94-5	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
Data File : BF118833.D
Acq On : 6 Feb 2020 12:22
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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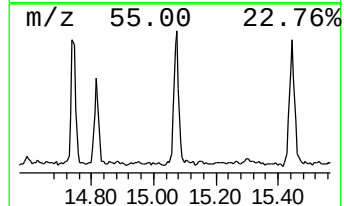
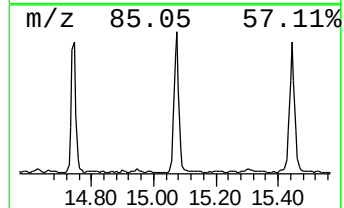
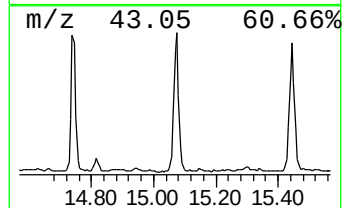
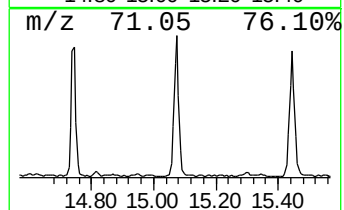
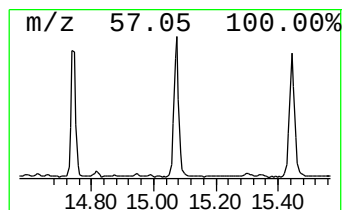
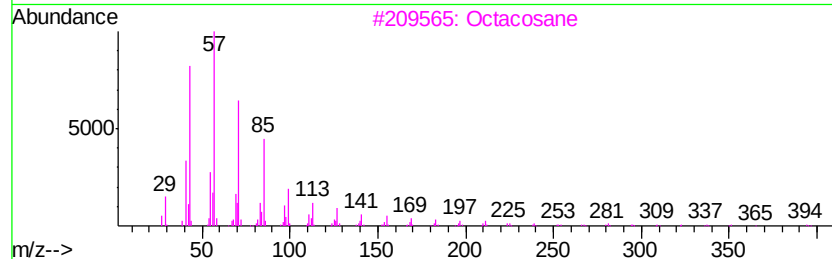
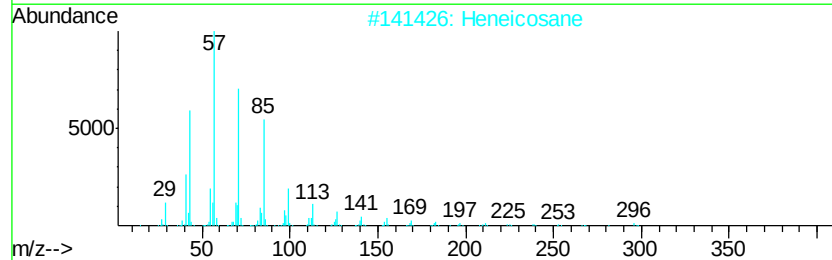
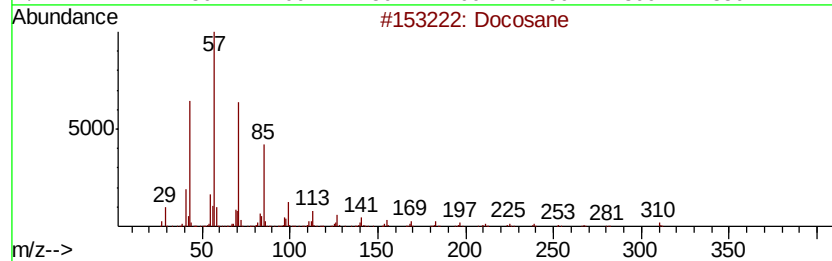
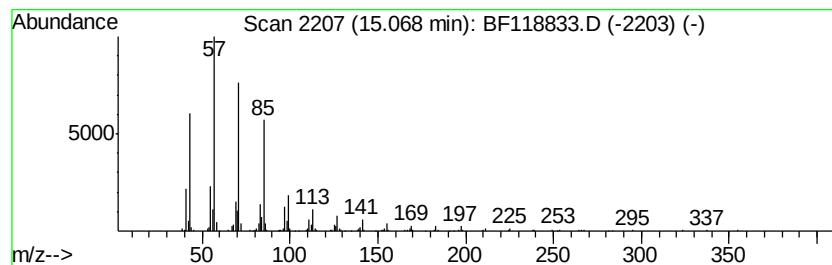
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Docosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	6.38 ng	616161	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Docosane	310	C22H46	000629-97-0	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Octadecane	254	C18H38	000593-45-3	91
5		Heptadecane	240	C17H36	000629-78-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
Data File : BF118833.D
Acq On : 6 Feb 2020 12:22
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

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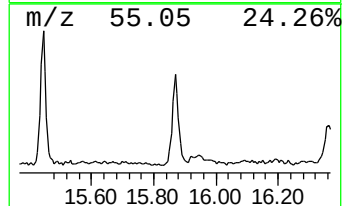
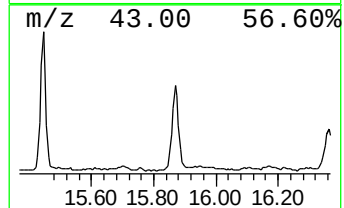
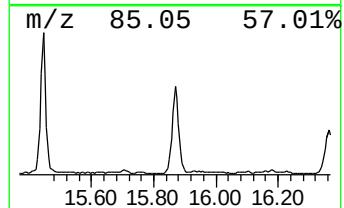
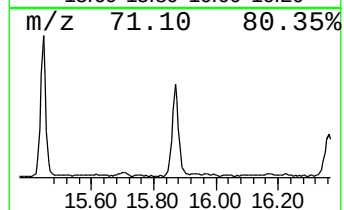
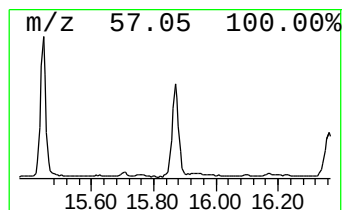
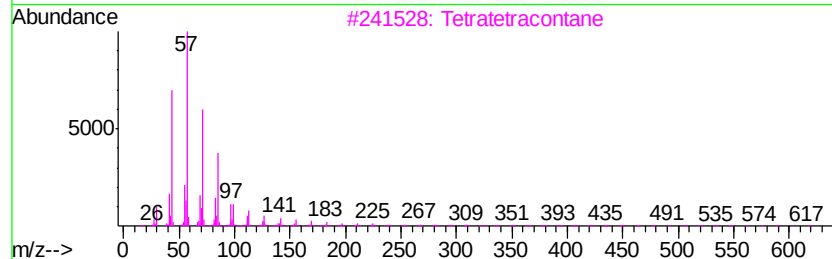
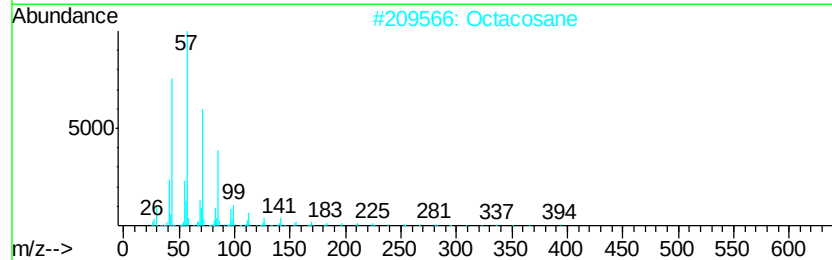
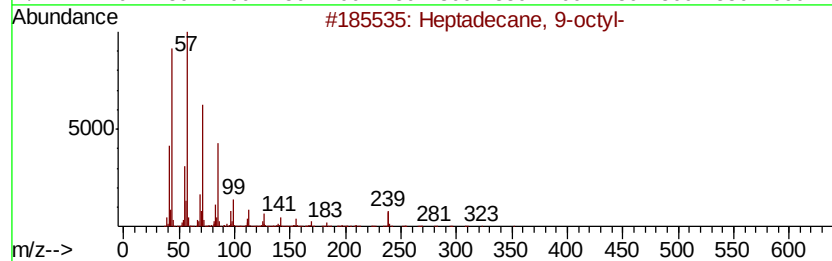
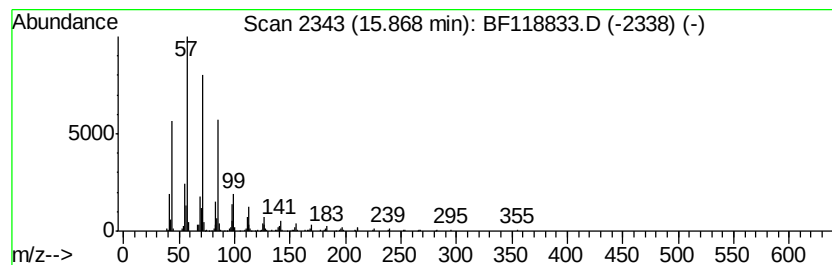
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	4.90 ng	473574	Perylene-d12	15.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Tetratetracontane	619	C44H90	007098-22-8	91
4		2-methyloctacosane	408	C29H60	1000376-72-8	91
5		Heptacosane	380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF020620\
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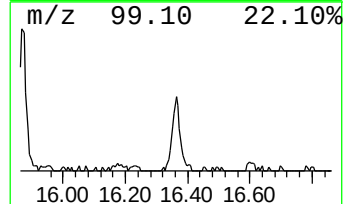
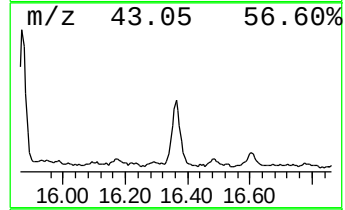
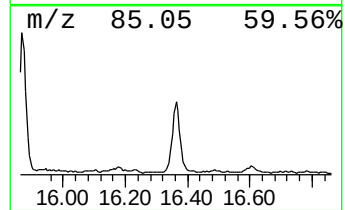
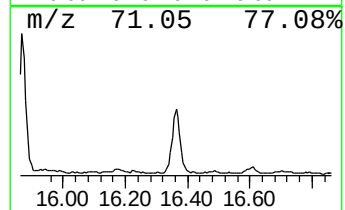
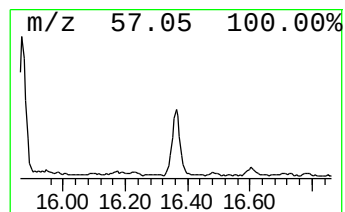
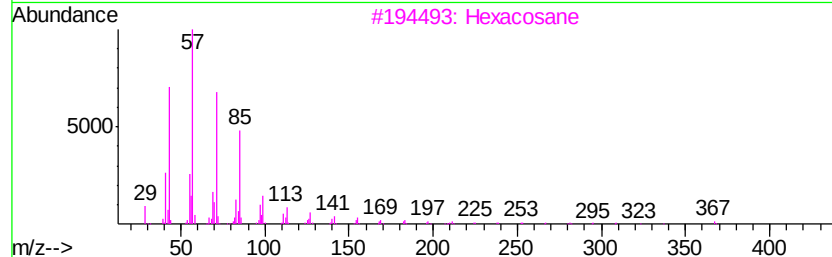
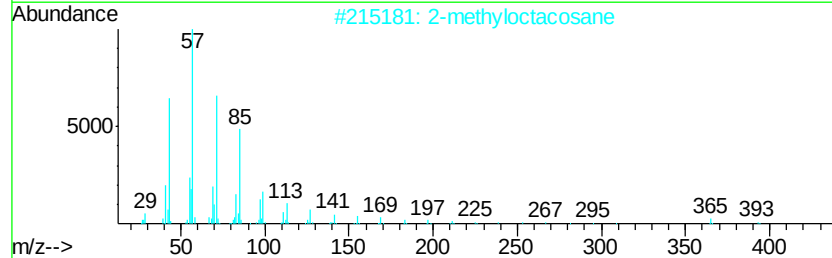
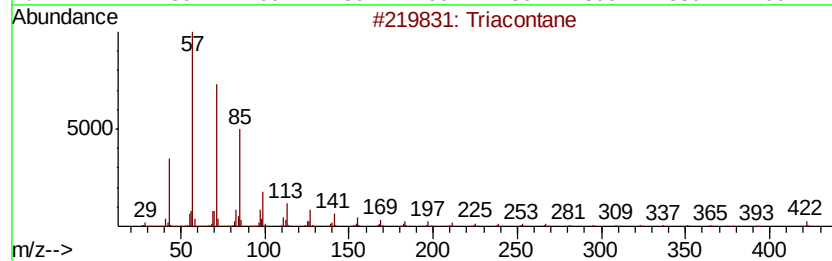
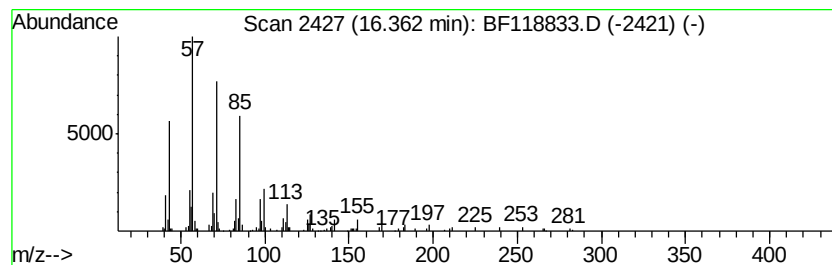
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.96 ng	286098	Perylene-d12	15.41
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triacontane	422 C30H62	000638-68-6 91
2		2-methyloctacosane	408 C29H60	1000376-72-8 91
3		Hexacosane	366 C26H54	000630-01-3 91
4		Pentadecane, 8-hexyl-	296 C21H44	013475-75-7 91
5		Heptadecane, 9-octyl-	352 C25H52	007225-64-1 91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF020620\
Data File : BF118833.D
Acq On : 6 Feb 2020 12:22
Operator : CG/JU
Sample : PB126588BL
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrameth...	9.29	5.4	ng	658379	3	9.85	2454940	20.0
n-Hexadecanoic acid	11.87	13.7	ng	1786930	4	11.33	2615490	20.0
Octadecanoic acid	12.64	5.4	ng	708856	4	11.33	2615490	20.0
Oxalic acid, isob...	13.82	6.3	ng	727669	5	13.97	2326720	20.0
Triacontane	14.14	2.1	ng	242552	5	13.97	2326720	20.0
2-methyloctacosane	14.44	3.8	ng	445013	5	13.97	2326720	20.0
Octadecane	14.74	5.4	ng	525166	6	15.41	1931260	20.0
Squalene	14.82	10.5	ng	1014090	6	15.41	1931260	20.0
Docosane	15.07	6.4	ng	616161	6	15.41	1931260	20.0
Heptadecane, 9-oc...	15.87	4.9	ng	473574	6	15.41	1931260	20.0
Hexacosane	16.36	3.0	ng	286098	6	15.41	1931260	20.0