

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042020\
 Data File : BF120082.D
 Acq On : 20 Apr 2020 17:18
 Operator : MA/SJ
 Sample : L2314-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-3-1

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-BF040820.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	5.316	544	549	552	rBV	3262404	3319083	75.89%	9.418%
2	6.357	720	726	729	rBV	3132192	3435614	78.55%	9.749%
3	6.545	754	758	763	rBV2	73229	71568	1.64%	0.203%
4	6.710	783	786	790	rBV	1086062	937912	21.44%	2.661%
5	6.869	809	813	816	rBV	3270550	2952385	67.50%	8.378%
6	7.122	849	856	859	rBV	71900	58620	1.34%	0.166%
7	7.281	874	883	886	rBV	2516978	2499150	57.14%	7.092%
8	7.998	1001	1005	1008	rBV	1484397	1296399	29.64%	3.679%
9	8.022	1008	1009	1012	rVB	164761	75737	1.73%	0.215%
10	8.710	1122	1126	1130	rBV	66469	57122	1.31%	0.162%
11	9.081	1183	1189	1192	rBV	4972720	4373786	100.00%	12.411%
12	9.163	1199	1203	1207	rBV2	38480	53015	1.21%	0.150%
13	9.475	1252	1256	1259	rBV	767705	561733	12.84%	1.594%
14	9.510	1259	1262	1265	rVV	88232	69523	1.59%	0.197%
15	9.757	1297	1304	1307	rBV	1664751	1352051	30.91%	3.837%
16	10.545	1433	1438	1441	rBV	2654264	2453612	56.10%	6.962%
17	10.669	1455	1459	1464	rBV2	48496	63464	1.45%	0.180%
18	11.239	1552	1556	1559	rBV	1431867	1293484	29.57%	3.670%
19	11.263	1559	1560	1563	rVB	141433	84275	1.93%	0.239%
20	11.692	1630	1633	1637	rBV	47486	54131	1.24%	0.154%
21	11.739	1637	1641	1644	rBV2	63844	72424	1.66%	0.206%
22	11.780	1644	1648	1653	rBV2	576627	544306	12.44%	1.545%
23	12.039	1687	1692	1694	rBV3	59358	75891	1.74%	0.215%
24	12.451	1759	1762	1766	rBV	150062	136841	3.13%	0.388%
25	12.563	1776	1781	1789	rBV2	247280	294358	6.73%	0.835%
26	12.680	1798	1801	1804	rVB	141851	112336	2.57%	0.319%
27	12.833	1822	1827	1830	rBV	4125244	3844486	87.90%	10.909%
28	13.257	1896	1899	1902	rVB	188469	146319	3.35%	0.415%
29	13.410	1923	1925	1929	rVB	80751	68580	1.57%	0.195%
30	13.504	1938	1941	1943	rBV3	66840	65142	1.49%	0.185%
31	13.621	1958	1961	1966	rBV4	57369	66394	1.52%	0.188%
32	13.739	1977	1981	1991	rVB2	285648	366040	8.37%	1.039%
33	13.880	2001	2005	2008	rBV	1069715	1072799	24.53%	3.044%
34	14.051	2031	2034	2038	rBV2	152818	149097	3.41%	0.423%

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 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 >
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35	14.092	2039	2041	2043	rBV	66477	54730	1.25%	0.155%
36	14.198	2057	2059	2062	rVB	60028	55399	1.27%	0.157%
37	14.245	2065	2067	2069	rBV	57274	59143	1.35%	0.168%
38	14.274	2069	2072	2074	rBV	171880	206712	4.73%	0.587%
39	14.333	2080	2082	2085	rBV	119555	94305	2.16%	0.268%
40	14.363	2085	2087	2089	rBV	78369	83389	1.91%	0.237%
41	14.404	2092	2094	2100	rVB2	123259	185744	4.25%	0.527%
42	14.521	2111	2114	2118	rVB	109064	101644	2.32%	0.288%
43	14.645	2132	2135	2141	rBV2	143196	209696	4.79%	0.595%
44	14.710	2143	2146	2154	rVB	175494	200205	4.58%	0.568%
45	14.898	2175	2178	2187	rVB	117156	227600	5.20%	0.646%
46	14.980	2189	2192	2199	rVB2	113118	145483	3.33%	0.413%
47	15.245	2234	2237	2242	rVB	98209	120145	2.75%	0.341%
48	15.310	2243	2248	2252	rBV	736422	993352	22.71%	2.819%
49	16.339	2420	2423	2428	rVB	71590	106884	2.44%	0.303%
50	16.680	2478	2481	2487	rVB3	48325	78068	1.78%	0.222%
51	17.098	2549	2552	2559	rVB3	46834	90512	2.07%	0.257%
52	18.527	2788	2795	2796	rBV3	71113	150378	3.44%	0.427%

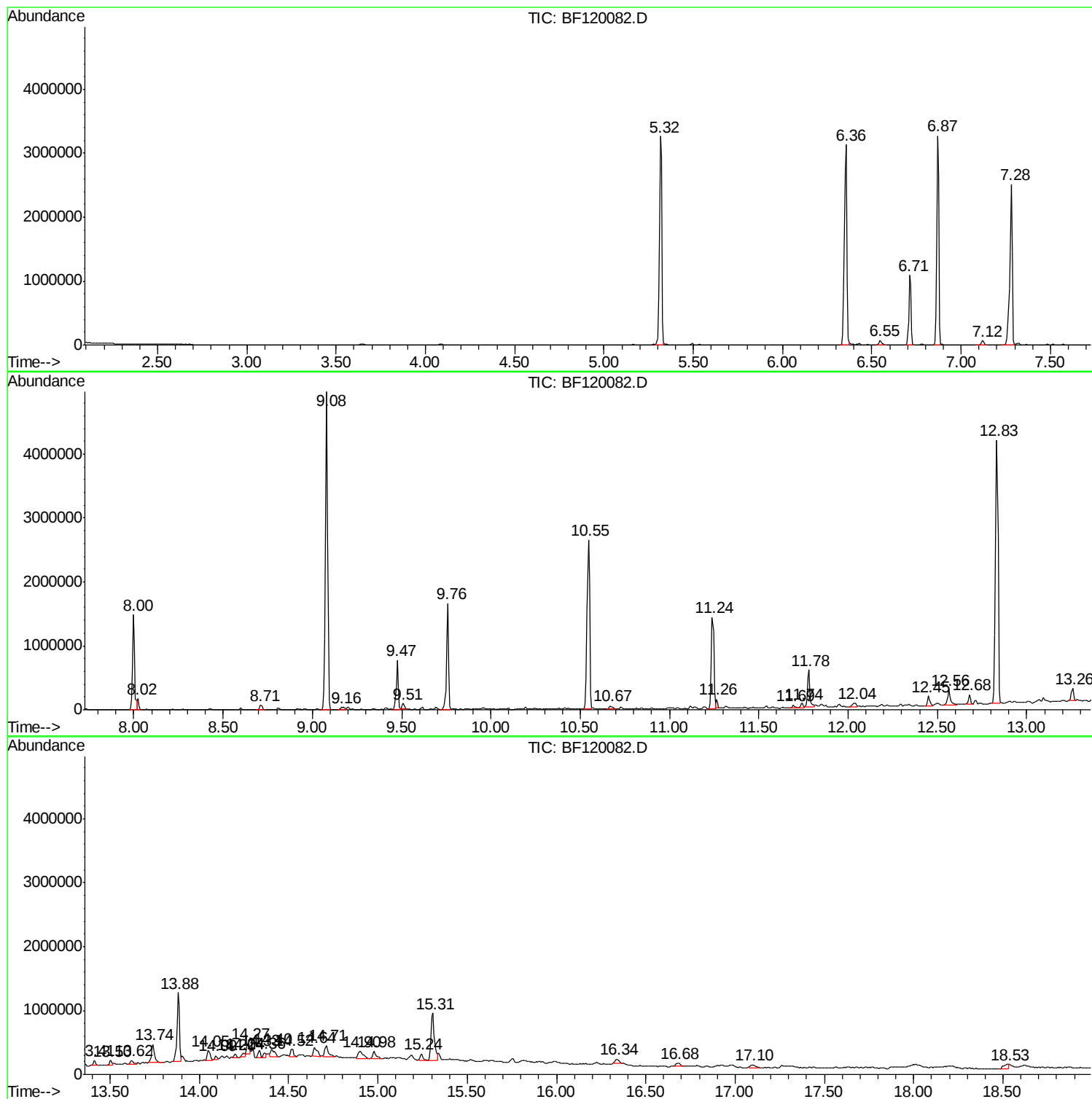
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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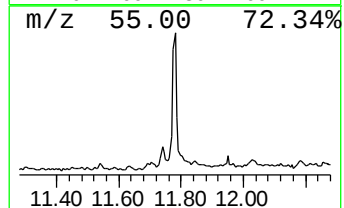
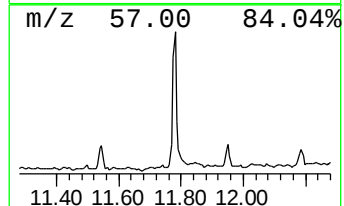
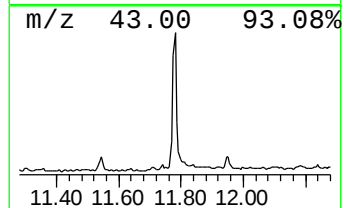
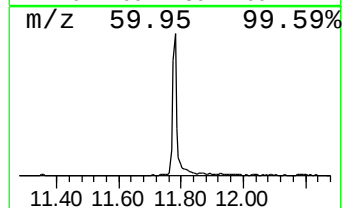
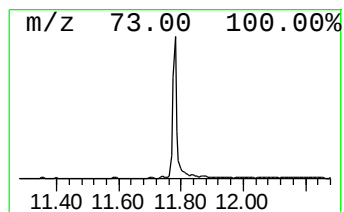
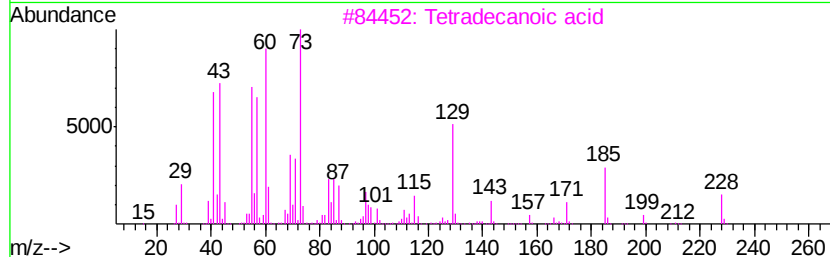
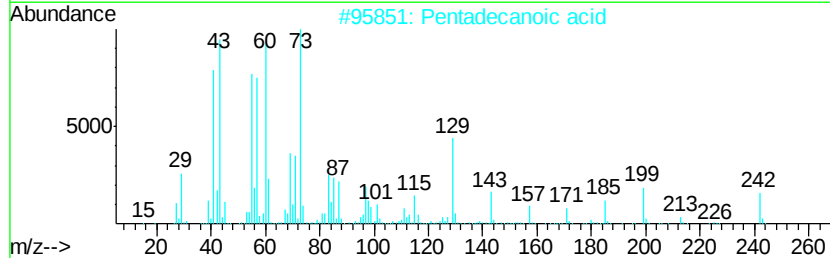
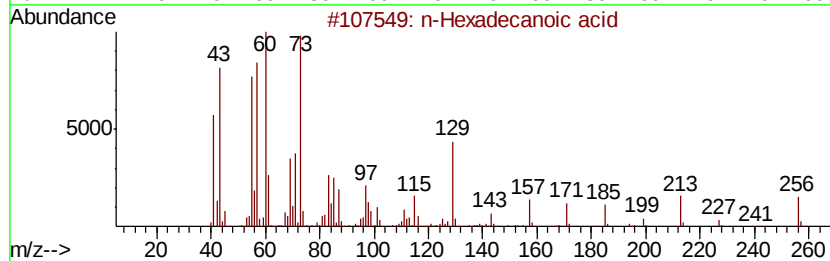
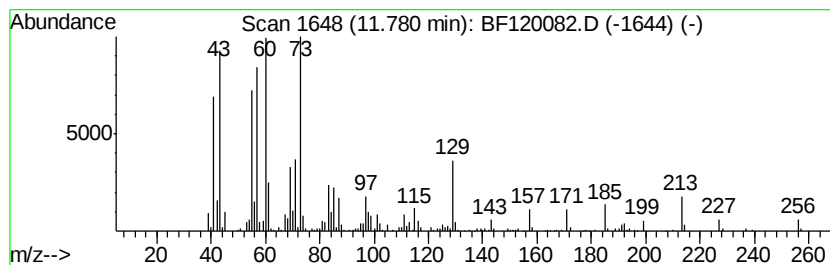
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	8.42 ng	544306	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60



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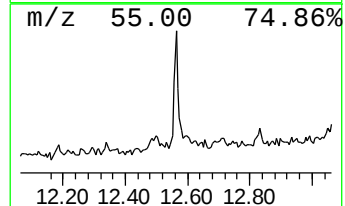
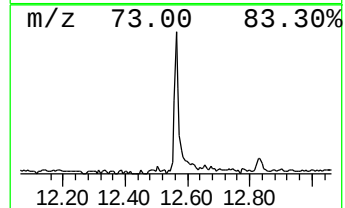
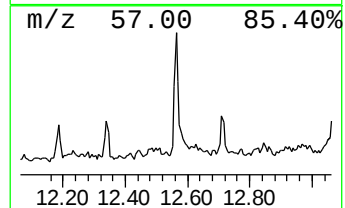
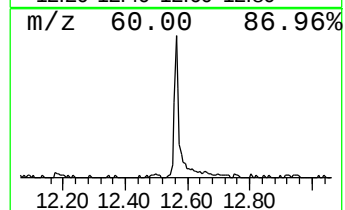
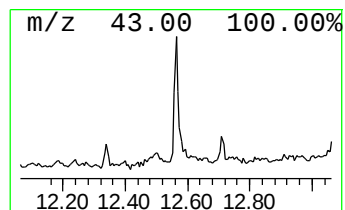
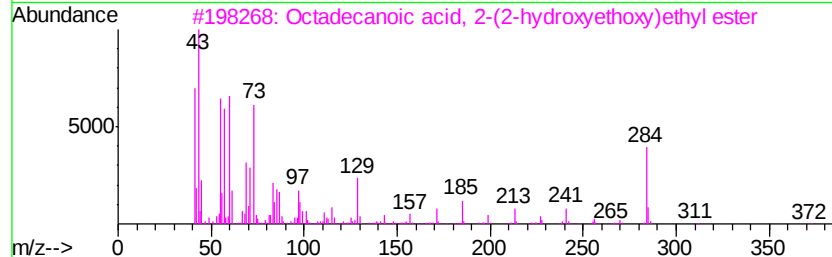
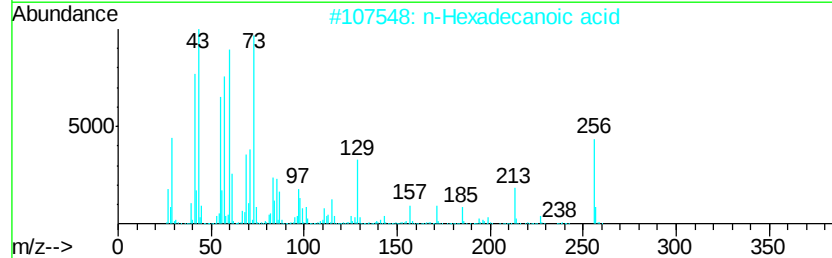
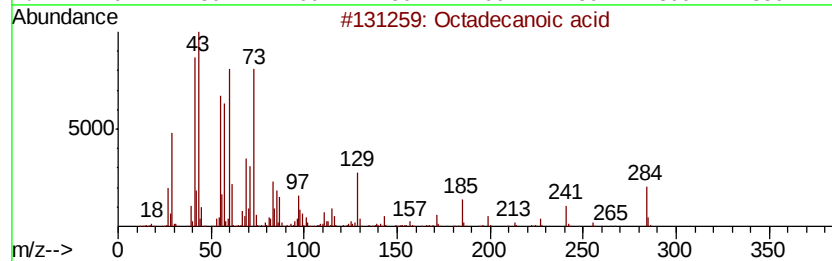
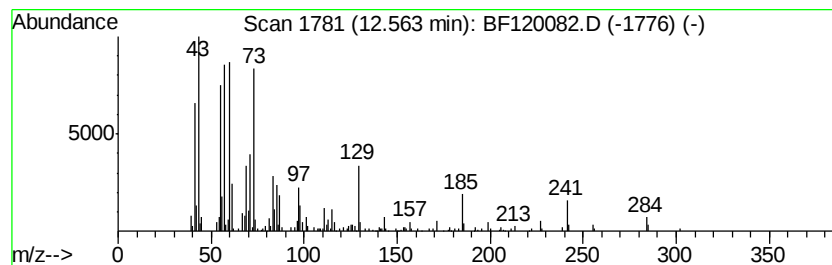
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	5.49 ng	294358	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3		Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5		Undecanoic acid	186	C11H22O2	000112-37-8	72



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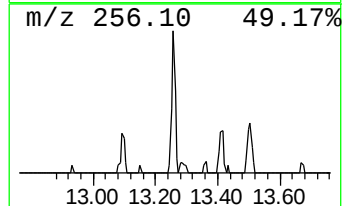
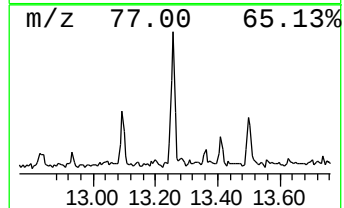
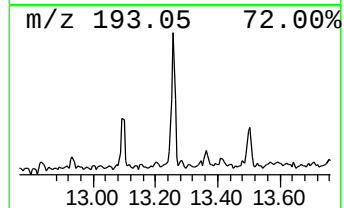
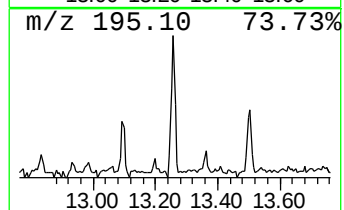
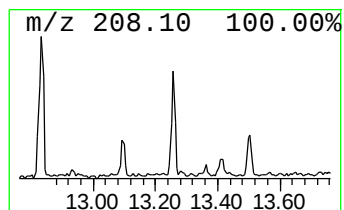
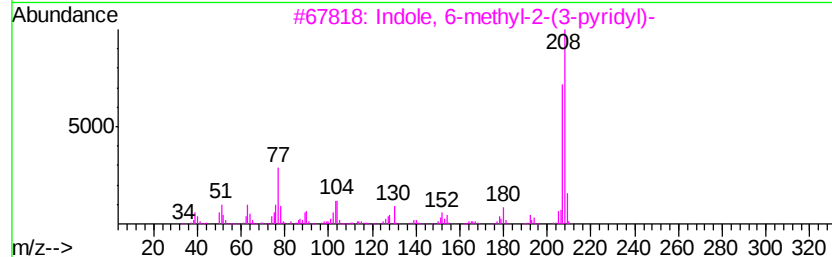
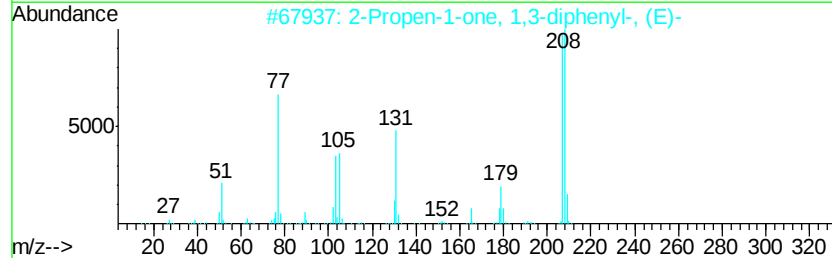
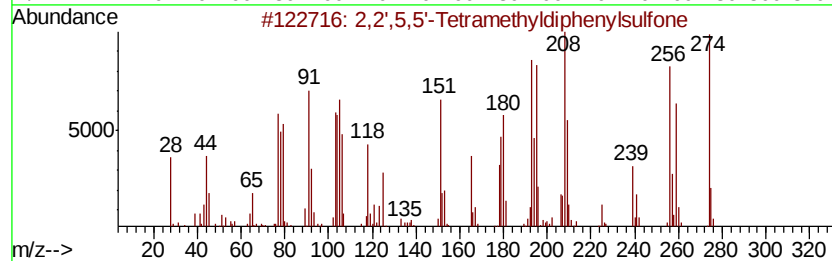
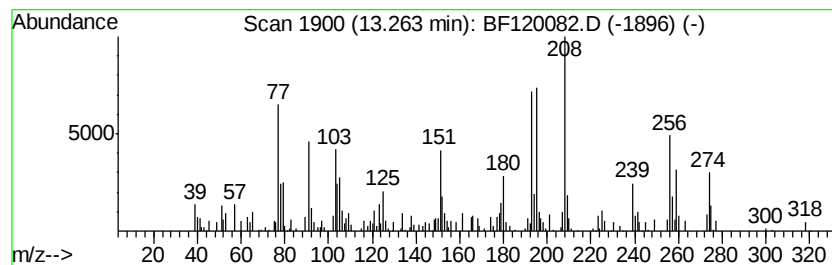
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2,2',5,5'-Tetramethyldiphen... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.26	2.73 ng	146319	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,2',5,5'-Tetramethyldiphenylsul...	274	C16H18O2S	006632-44-6	58
2		2-Propen-1-one, 1,3-diphenyl-, (E)-	208	C15H12O	000614-47-1	42
3		Indole, 6-methyl-2-(3-pyridyl)-	208	C14H12N2	293762-69-3	27
4		2,2',4,4'-Tetramethyldiphenylsul...	274	C16H18O2S	005184-75-8	25
5		Thiazolo[3,2-a]pyrimidin-7(7H)-o...	208	C10H12N2OS	1000270-11-6	22



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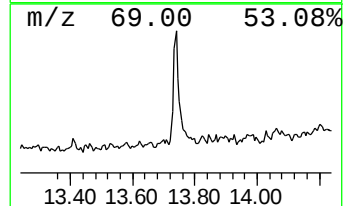
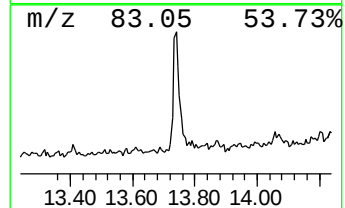
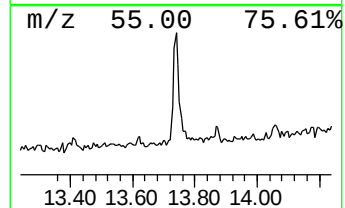
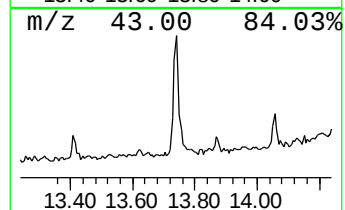
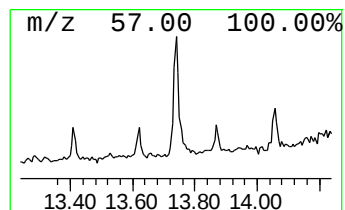
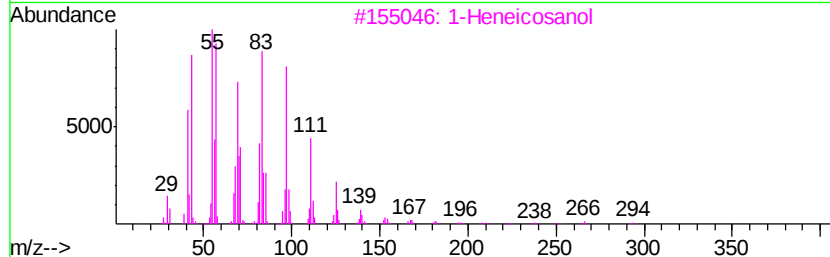
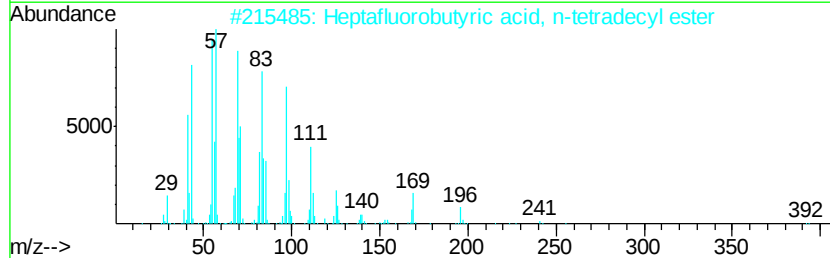
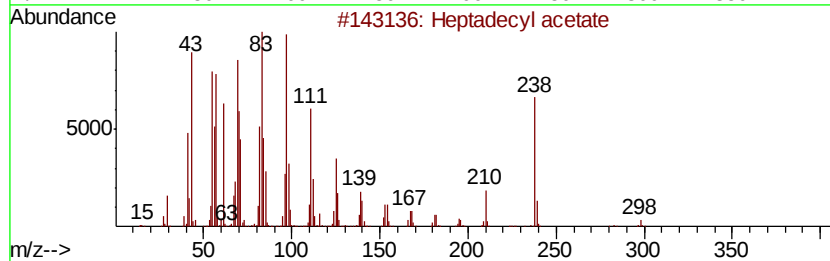
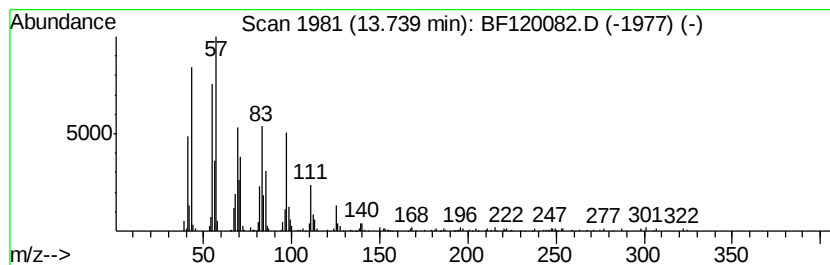
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptadecyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	6.82 ng	366040	Chrysene-d12	13.88

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl acetate	298	C19H38O2	000822-20-8	94
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
3		1-Heneicosanol	312	C21H44O	015594-90-8	91
4		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	91



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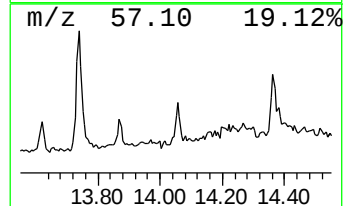
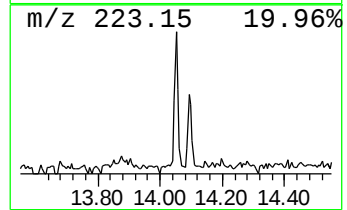
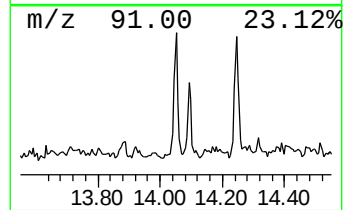
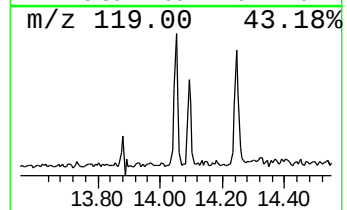
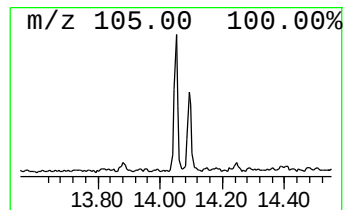
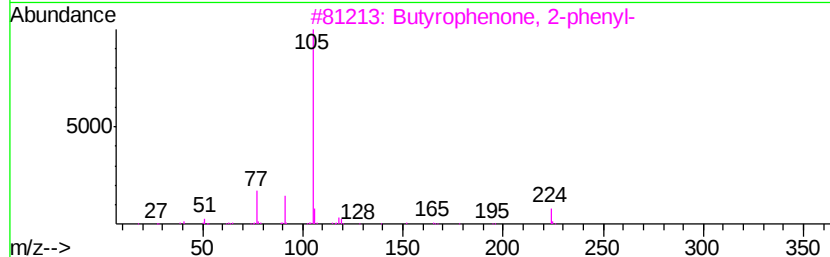
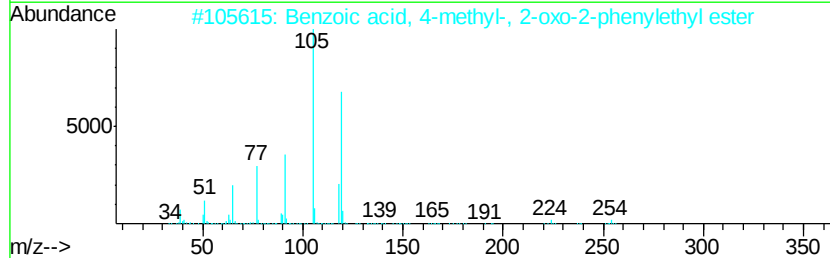
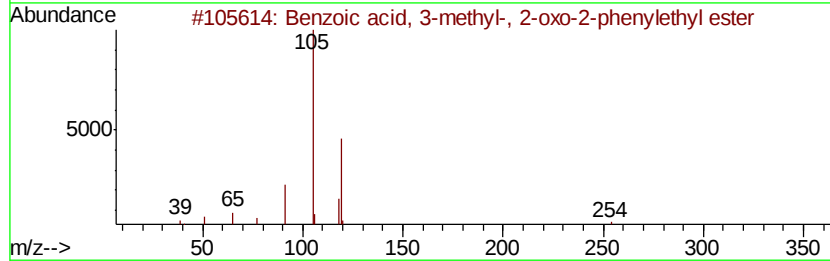
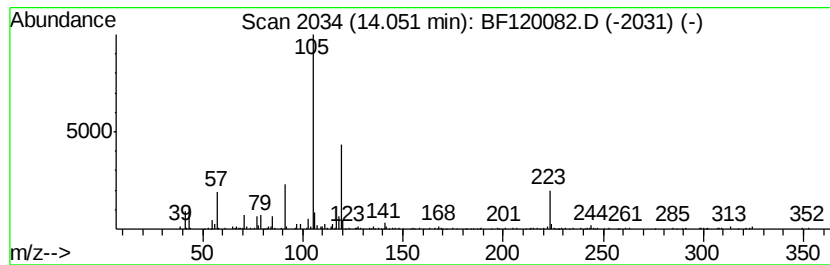
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.05 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.78 ng	149097	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 3-methyl-, 2-oxo-2...	254	C16H14O3	055153-20-3	28
2		Benzoic acid, 4-methyl-, 2-oxo-2...	254	C16H14O3	054797-44-3	23
3		Butyrophenone, 2-phenyl-	224	C16H16O	016282-16-9	14
4		Benzoic acid, N'-[(ethylamino)ca...	223	C10H13N3OS	1000327-65-8	12
5		Acetohydrazide, 2-cyano-N2-[4-(4...	307	C18H17N3O2	1000259-83-5	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042020\
Data File : BF120082.D
Acq On : 20 Apr 2020 17:18
Operator : MA/SJ
Sample : L2314-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

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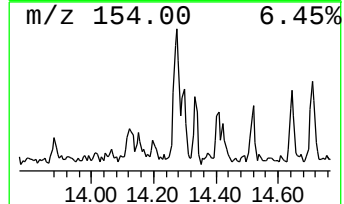
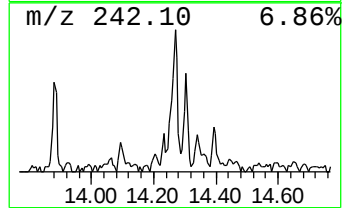
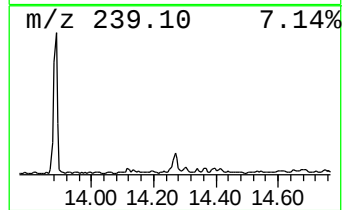
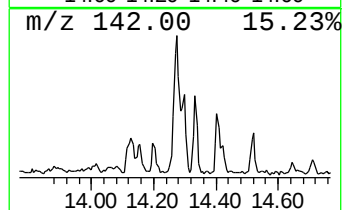
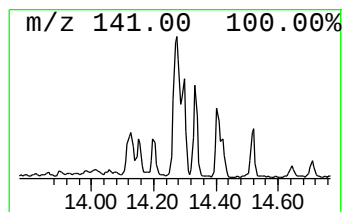
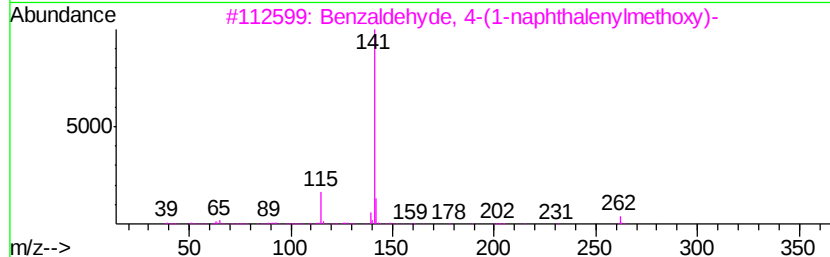
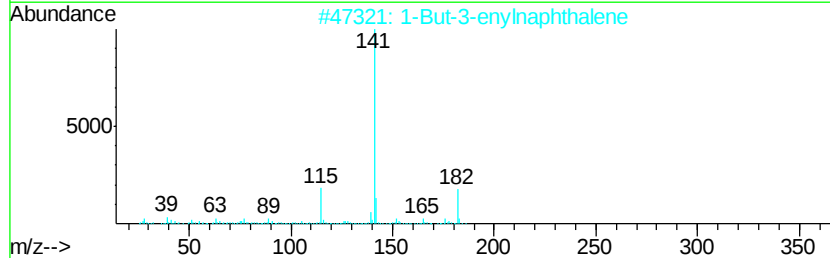
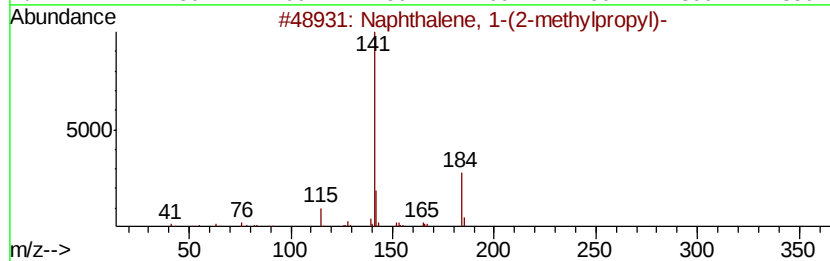
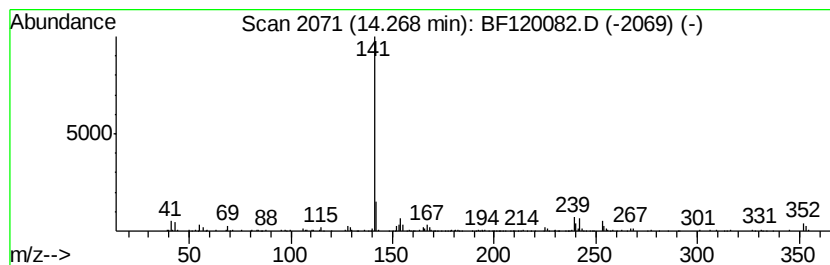
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Naphthalene, 1-(2-methylpro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.27	3.85 ng	206712	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	59
2		1-But-3-enylnaphthalene	182	C14H14	002489-88-5	45
3		Benzaldehyde, 4-(1-naphthalenylm...)	262	C18H14O2	1000338-23-3	38
4		Naphthalene, 1-propyl-	170	C13H14	002765-18-6	38
5		Pyrazol-4-amine, 3,5-dimethyl-1-...	251	C16H17N3	1000273-77-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042020\
Data File : BF120082.D
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Misc :
ALS Vial : 11 Sample Multiplier: 1

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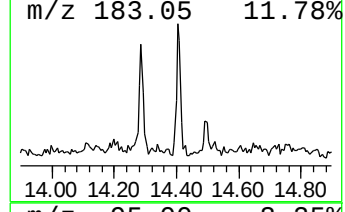
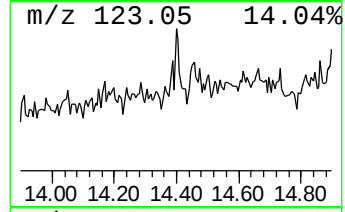
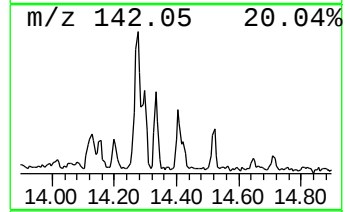
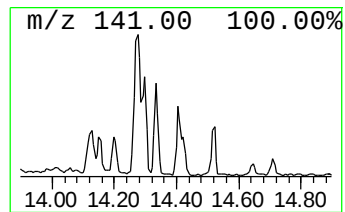
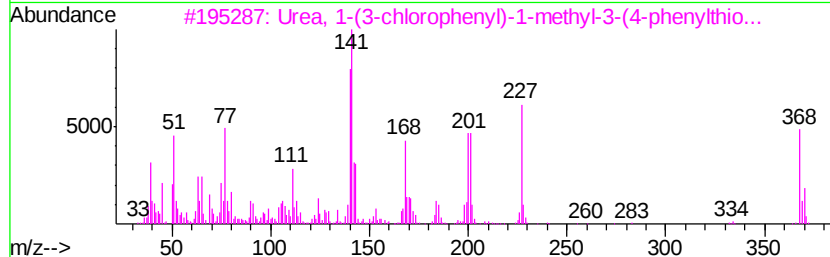
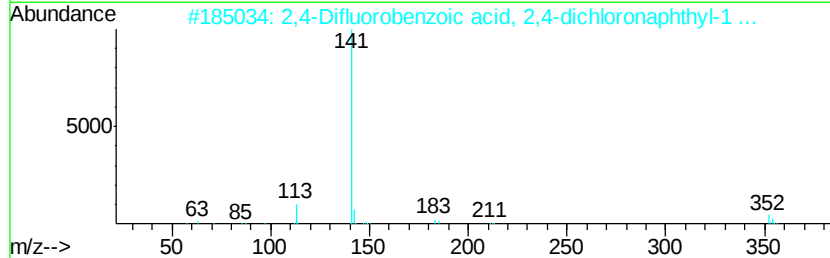
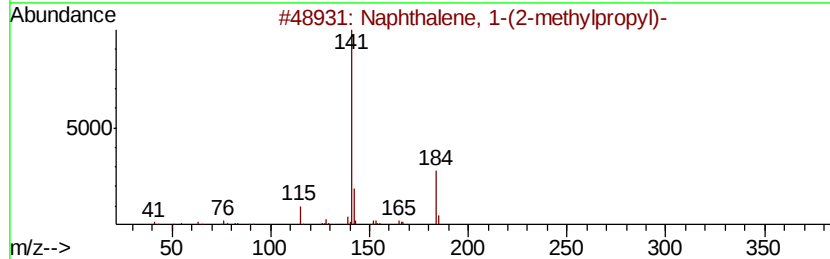
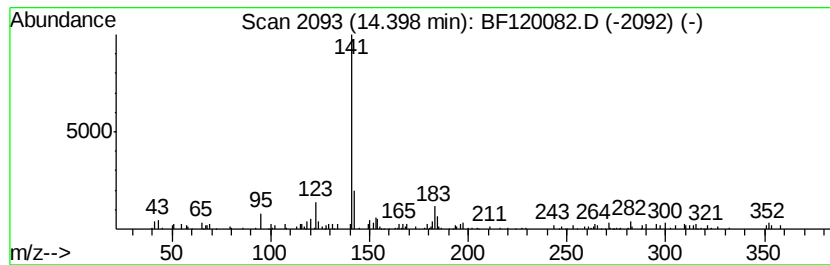
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2,4-Difluorobenzoic acid, 2... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	3.46 ng	185744	Chrysene-d12	13.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-(2-methylpropyl)-	184	C14H16	016727-91-6	64
2		2,4-Difluorobenzoic acid, 2,4-di...	352	C17H8Cl2F2O2	1000331-58-5	50
3		Urea, 1-(3-chlorophenyl)-1-methyl...	368	C20H17ClN2OS	1000296-25-3	46
4		1-But-3-enyl-naphthalene	182	C14H14	002489-88-5	45
5		1-Pyridineacetic acid, 4-(aminoc...	326	C18H34N2O3	1000319-12-3	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042020\
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Acq On : 20 Apr 2020 17:18
Operator : MA/SJ
Sample : L2314-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

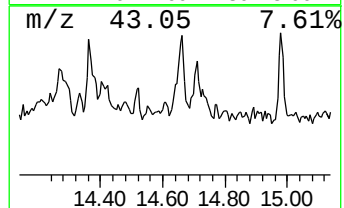
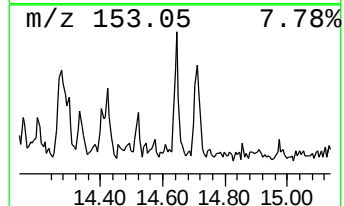
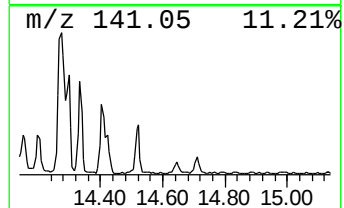
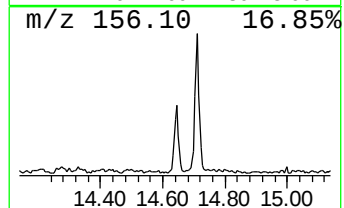
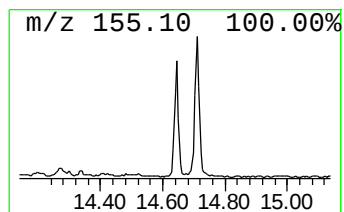
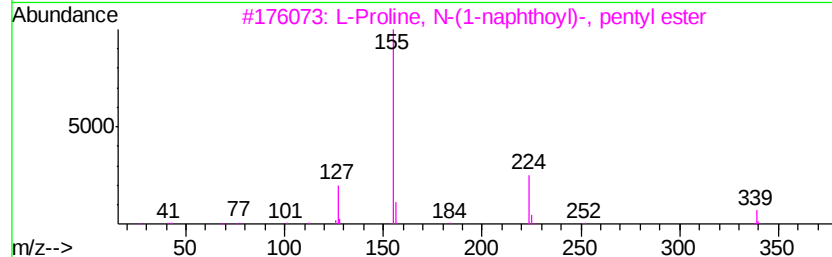
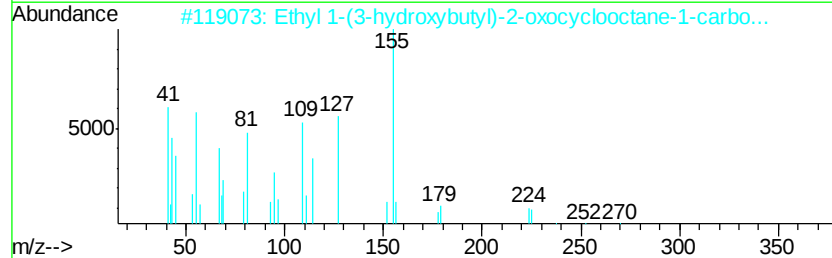
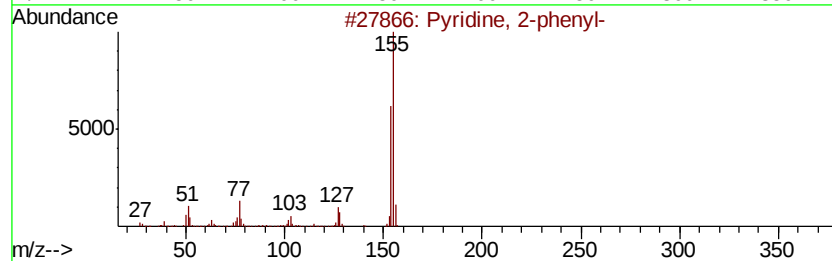
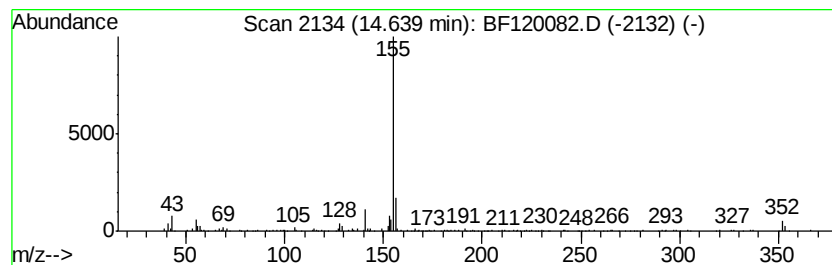
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF040820.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Pyridine, 2-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.22 ng	209696	Perylene-d12	15.31
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyridine, 2-phenyl-	155 C11H9N	001008-89-5 59
2		Ethyl 1-(3-hydroxybutyl)-2-oxocy...	270 C15H26O4	110288-16-9 58
3		L-Proline, N-(1-naphthovl)-, pen...	339 C21H25N03	1000346-08-6 53
4		Fumaric acid, butyl 3,5-difluoro...	284 C14H14F2O4	1000339-37-0 53
5		1,6-Anhydro-2,3-O-isopropylidene...	316 C15H28O5Si	1000364-42-4 53



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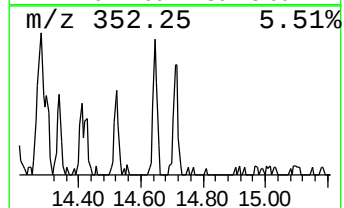
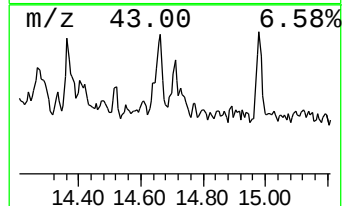
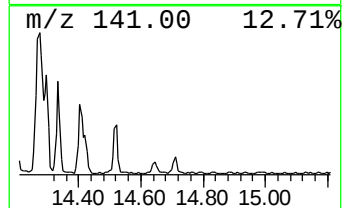
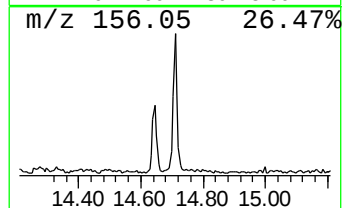
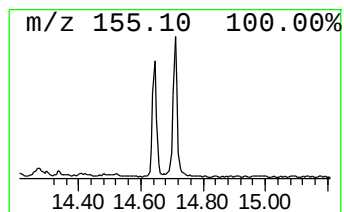
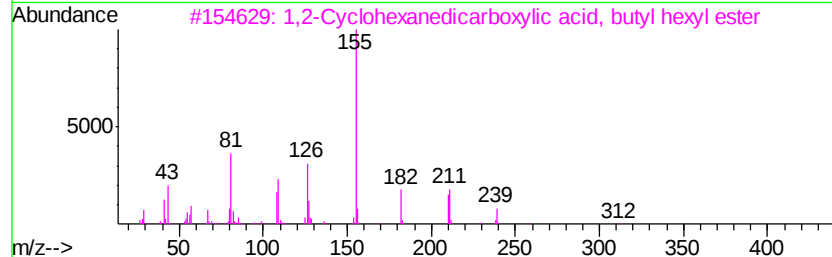
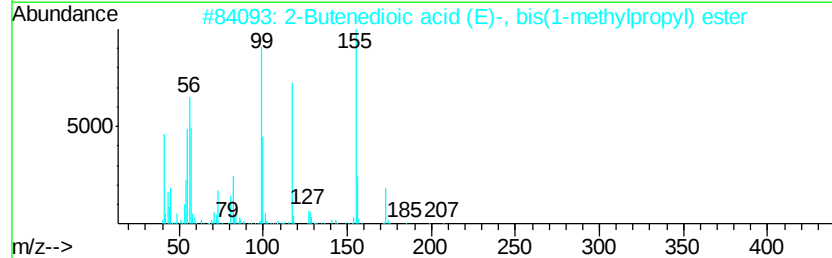
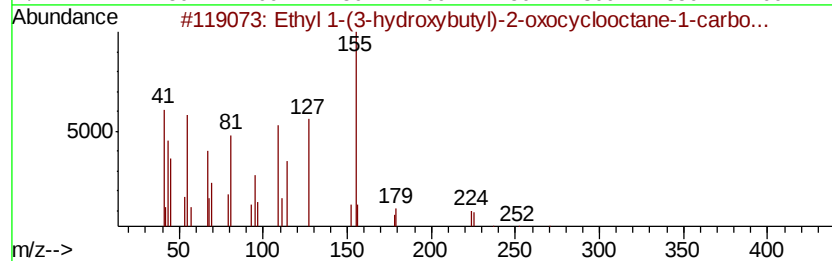
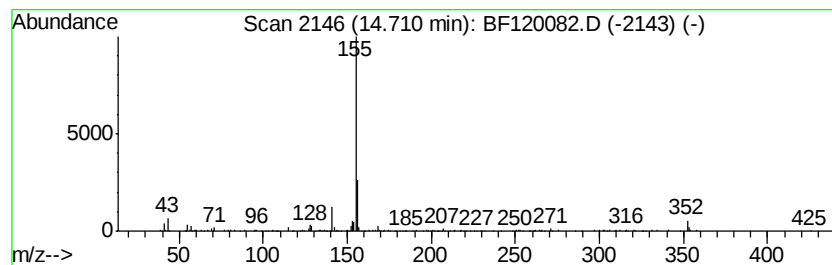
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Ethyl 1-(3-hydroxybutyl)-2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	4.03 ng	200205	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl 1-(3-hydroxybutyl)-2-oxocyclooctane-1-carboxylate	270	C15H26O4	110288-16-9	50
2		2-Butenedioic acid (E)-, bis(1-methylpropyl) ester	228	C12H20O4	002210-32-4	38
3		1,2-Cyclohexanedicarboxylic acid, butyl hexyl ester	312	C18H32O4	1000339-40-9	33
4		1,2-Cyclohexanedicarboxylic acid, butyl hexyl ester	312	C18H32O4	1000339-42-7	33
5		1-Naphthoic acid, 2,4,6-trichloro-3-methyl	350	C17H9Cl3O2	1000325-54-3	28



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042020\
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Acq On : 20 Apr 2020 17:18
Operator : MA/SJ
Sample : L2314-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

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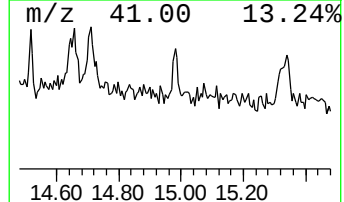
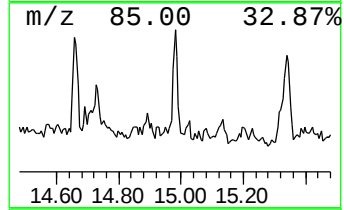
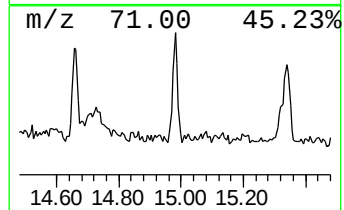
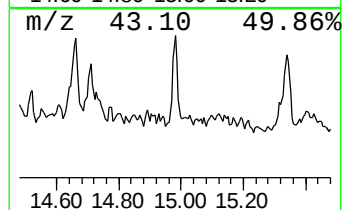
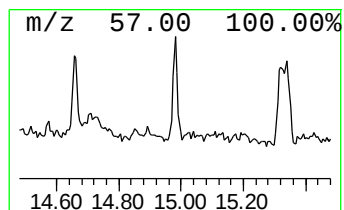
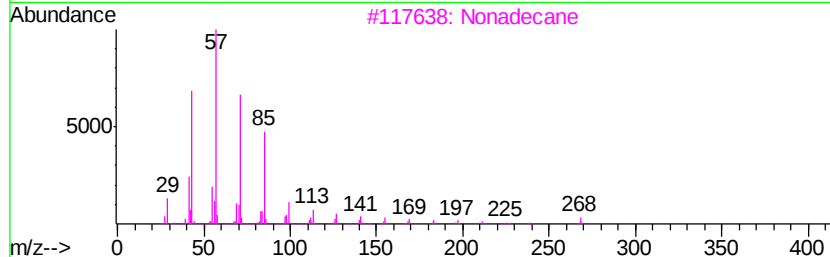
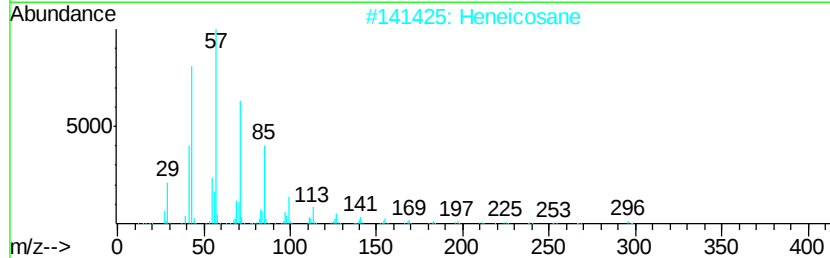
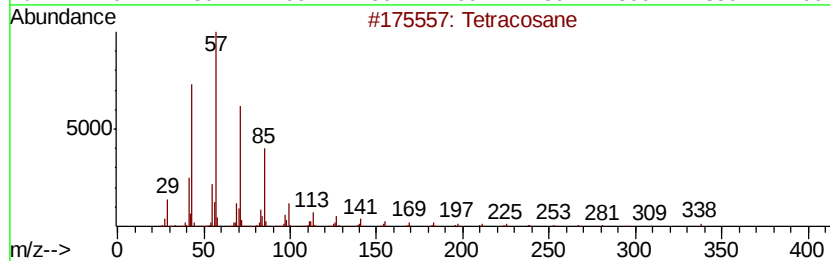
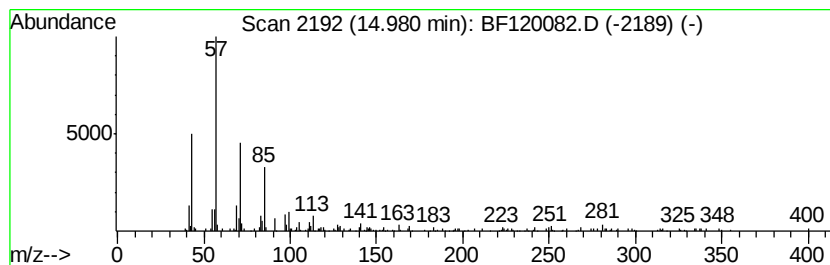
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Tetracosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.93 ng	145483	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	96
2		Heneicosane	296	C21H44	000629-94-7	96
3		Nonadecane	268	C19H40	000629-92-5	96
4		Hexadecane	226	C16H34	000544-76-3	95
5		Octacosane	394	C28H58	000630-02-4	87



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Misc :
ALS Vial : 11 Sample Multiplier: 1

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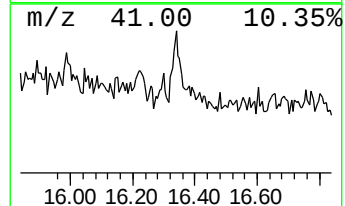
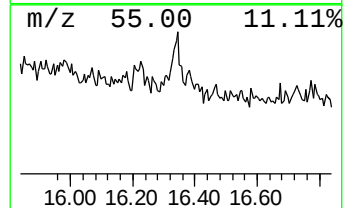
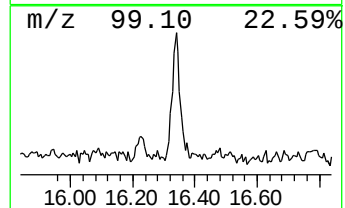
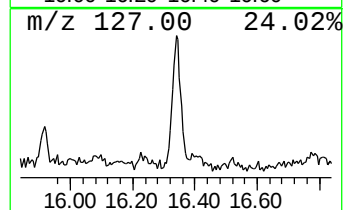
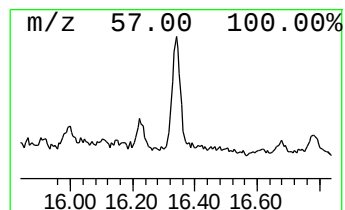
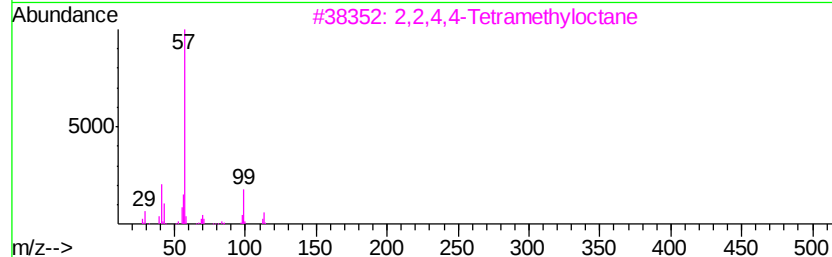
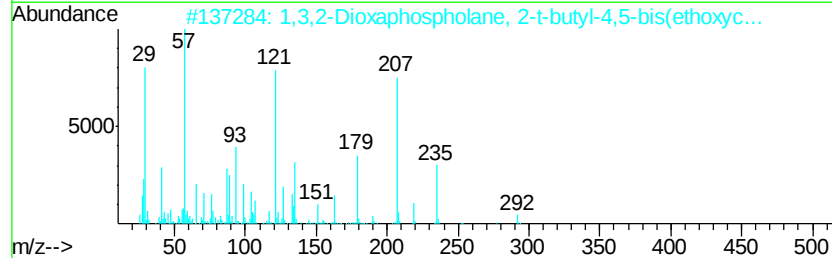
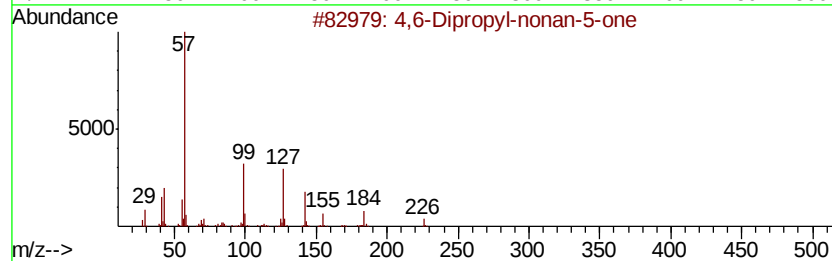
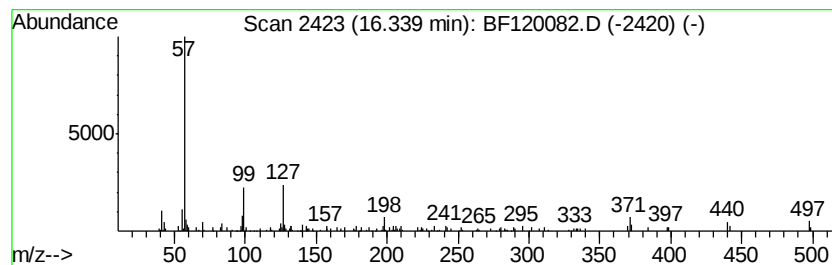
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 4,6-Dipropyl-nonan-5-one Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	2.15 ng	106884	Perylene-d12	15.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,6-Dipropyl-nonan-5-one	226	C15H30O	1000190-93-3	50
2			1,3,2-Dioxaphospholane, 2-t-butyl...	292	C12H21O6P	080043-97-6	40
3			2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	25
4			1-Hexanol, 2,2-dimethyl-	130	C8H18O	002370-13-0	17
5			Heptane, 3-(chloromethyl)-	148	C8H17Cl	000123-04-6	17



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042020\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WB-3-1

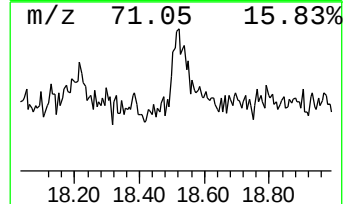
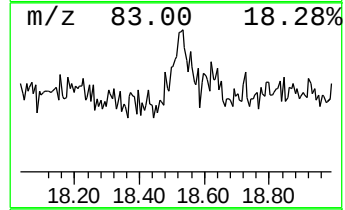
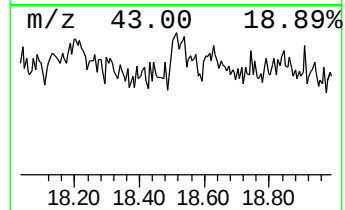
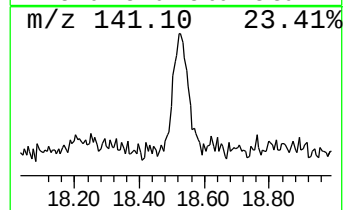
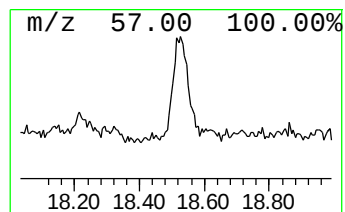
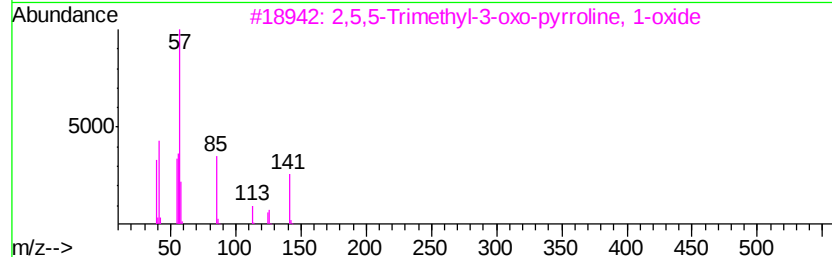
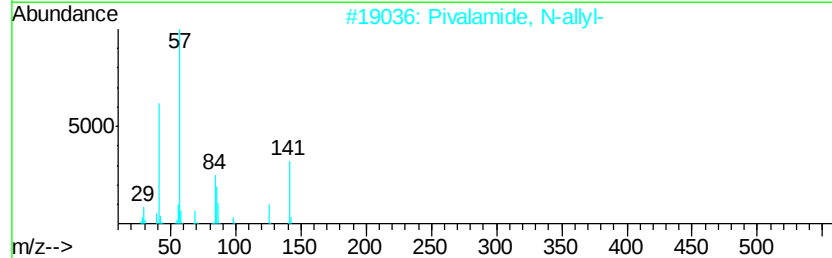
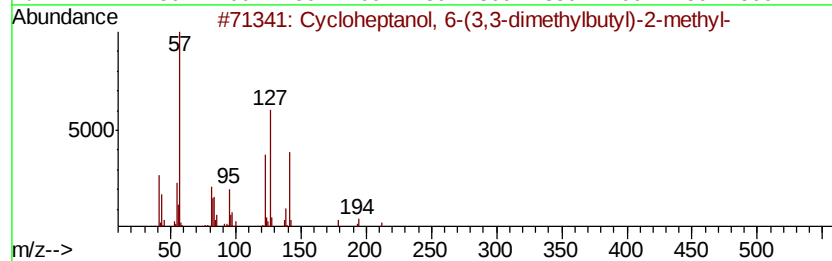
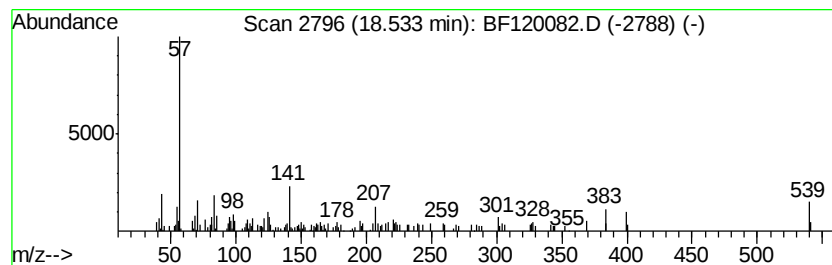
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown18.53 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.53	3.03 ng	150378	Perylene-d12	15.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloheptanol, 6-(3,3-dimethylbu...	212	C14H28O	040565-00-2	11
2		Pivalamide, N-allyl-	141	C8H15NO	1000345-72-4	9
3		2,5,5-Trimethyl-3-oxo-pyrroline,...	141	C7H11NO2	1000305-90-5	9
4		1-Azacyclononan-2-one	141	C8H15NO	000935-30-8	9
5		7-t-Butoxybicyclo[2.2.1]heptane-...	196	C11H16O3	1000210-03-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042020\
 Data File : BF120082.D
 Acq On : 20 Apr 2020 17:18
 Operator : MA/SJ
 Sample : L2314-03
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WB-3-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040820.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
n-Hexadecanoic acid	11.78	8.4 ng		544306	4	11.24	1293480	20.0
Octadecanoic acid	12.56	5.5 ng		294358	5	13.88	1072800	20.0
2,2',5,5'-Tetrame...	13.26	2.7 ng		146319	5	13.88	1072800	20.0
Heptadecyl acetate	13.74	6.8 ng		366040	5	13.88	1072800	20.0
unknown14.05	14.05	2.8 ng		149097	5	13.88	1072800	20.0
Naphthalene, 1-(2...	14.27	3.9 ng		206712	5	13.88	1072800	20.0
2,4-Difluorobenzo...	14.40	3.5 ng		185744	5	13.88	1072800	20.0
Pyridine, 2-phenyl-	14.64	4.2 ng		209696	6	15.31	993352	20.0
Ethyl 1-(3-hydrox...	14.71	4.0 ng		200205	6	15.31	993352	20.0
Tetracosane	14.98	2.9 ng		145483	6	15.31	993352	20.0
4,6-Dipropyl-nona...	16.34	2.1 ng		106884	6	15.31	993352	20.0
unknown18.53	18.53	3.0 ng		150378	6	15.31	993352	20.0