

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051920\
 Data File : BF120364.D
 Acq On : 19 May 2020 15:21
 Operator : MA/SJ
 Sample : L2686-02 2X
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-214

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-BF051420.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	5.198	525	529	550	rBV	1582478	2001583	68.83%	6.041%
2	6.251	705	708	735	rBV	1666148	2115062	72.73%	6.383%
3	6.592	762	766	778	rBV	1268914	1402642	48.23%	4.233%
4	6.745	788	792	808	rBV	1879231	1844300	63.42%	5.566%
5	7.163	859	863	875	rBV	1136637	1447343	49.77%	4.368%
6	7.881	979	985	992	rBV	1876177	1902361	65.41%	5.741%
7	8.580	1100	1104	1109	rVB	263322	234821	8.07%	0.709%
8	8.869	1151	1153	1155	rBV2	117569	108327	3.72%	0.327%
9	8.957	1164	1168	1173	rBV	2655855	2908177	100.00%	8.777%
10	9.033	1178	1181	1183	rBV3	287183	339967	11.69%	1.026%
11	9.086	1188	1190	1195	rVV3	226996	399768	13.75%	1.206%
12	9.310	1225	1228	1231	rBV	1182929	910846	31.32%	2.749%
13	9.504	1258	1261	1262	rBV2	814798	827749	28.46%	2.498%
14	9.551	1266	1269	1273	rVB2	1511906	1794470	61.70%	5.416%
15	9.639	1282	1284	1289	rVB	2152731	2111190	72.59%	6.371%
16	12.721	1806	1808	1816	rVB	1656649	1985896	68.29%	5.993%
17	13.762	1981	1985	1988	rBV3	1511287	2234725	76.84%	6.744%
18	13.792	1988	1990	1998	rVB	820105	833548	28.66%	2.516%
19	14.262	2067	2070	2074	rVB2	1288265	1371231	47.15%	4.138%
20	14.668	2137	2139	2148	rVB4	199862	234123	8.05%	0.707%
21	14.768	2152	2156	2165	rVV	875397	1569468	53.97%	4.737%
22	14.839	2165	2168	2171	rVV2	222590	298520	10.26%	0.901%
23	14.868	2171	2173	2179	rVB2	254768	311873	10.72%	0.941%
24	15.039	2199	2202	2207	rVB	480490	575079	19.77%	1.736%
25	15.098	2208	2212	2216	rVB	627686	760092	26.14%	2.294%
26	15.151	2217	2221	2224	rBV	1135485	1423313	48.94%	4.295%
27	16.468	2440	2445	2452	rVB2	375127	686578	23.61%	2.072%
28	16.862	2507	2512	2520	rVB	262741	502207	17.27%	1.516%

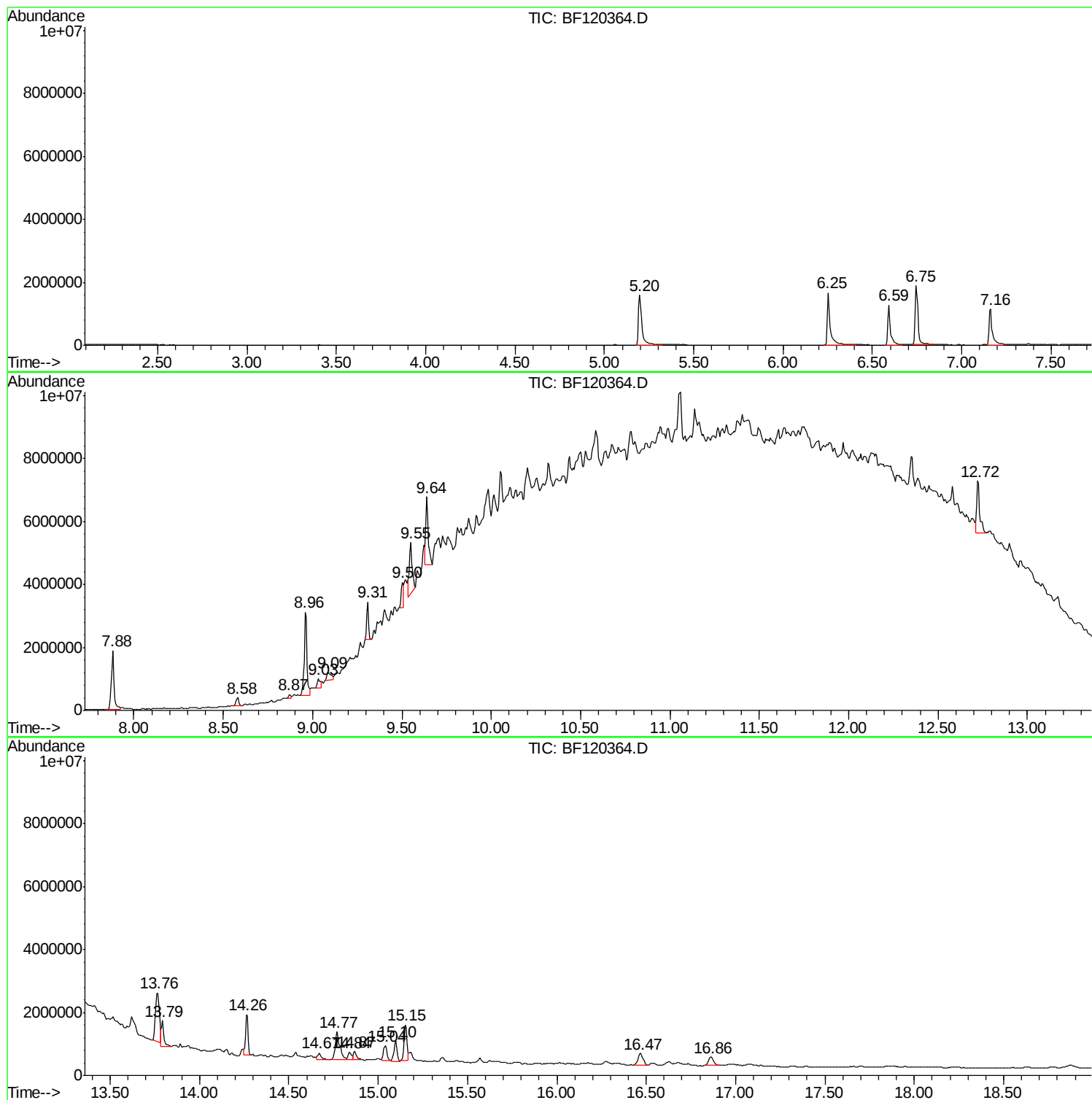
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Misc :
ALS Vial : 8 Sample Multiplier: 1

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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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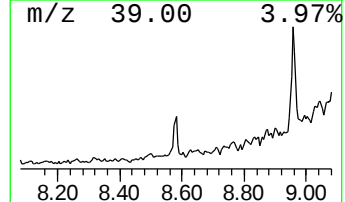
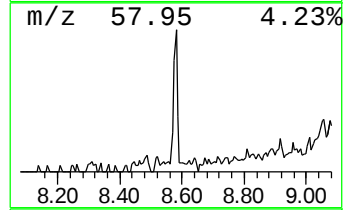
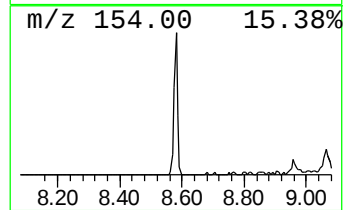
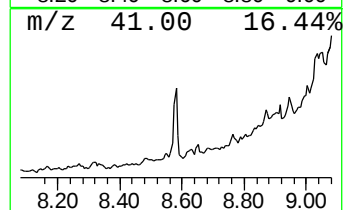
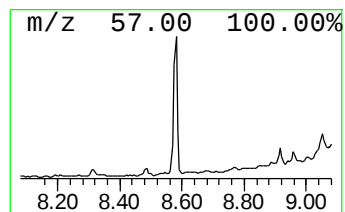
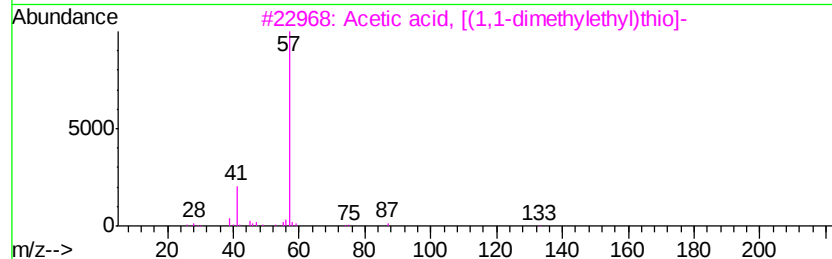
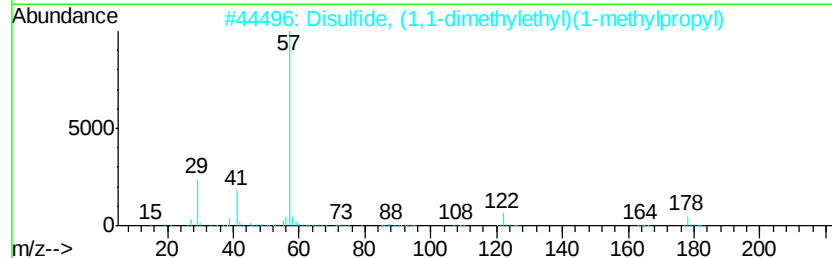
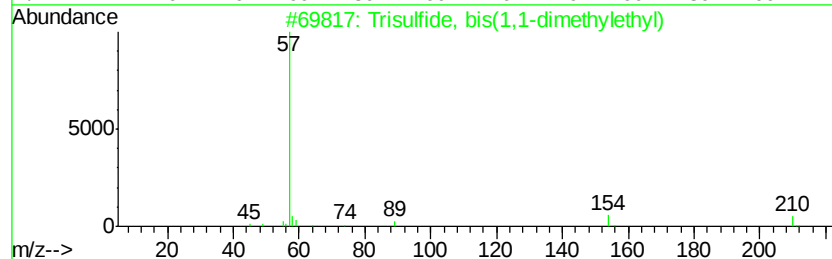
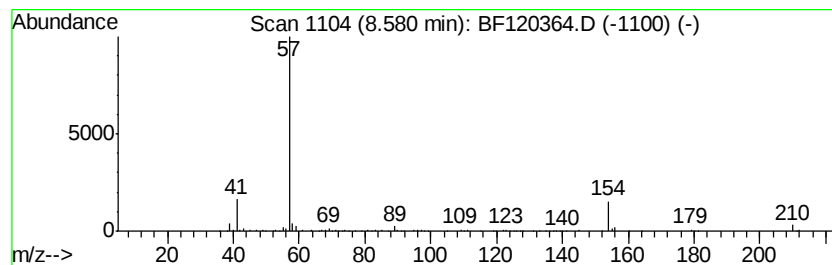
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Trisulfide, bis(1,1-dimethy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.58	2.47 ng	234821	Naphthalene-d8	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	72
2		Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	25
3		Acetic acid, [(1,1-dimethylethyl)...	148	C6H12O2S	024310-22-3	25
4		Isobutyl ether	130	C8H18O	000628-55-7	23
5		Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	23



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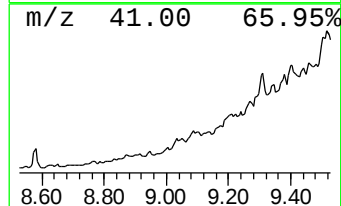
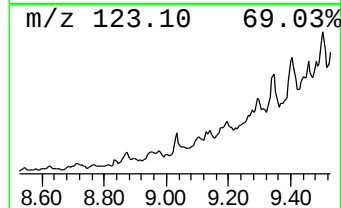
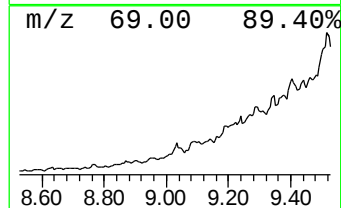
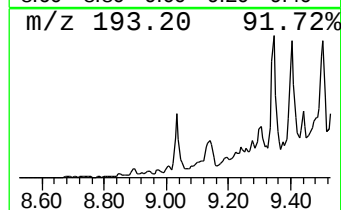
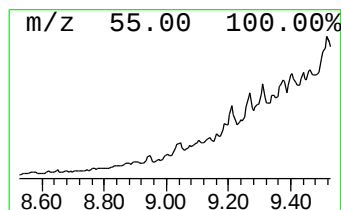
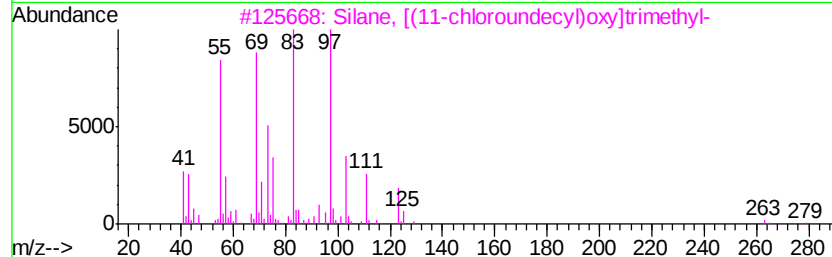
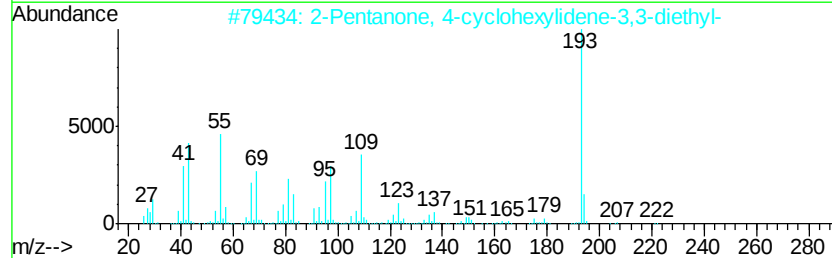
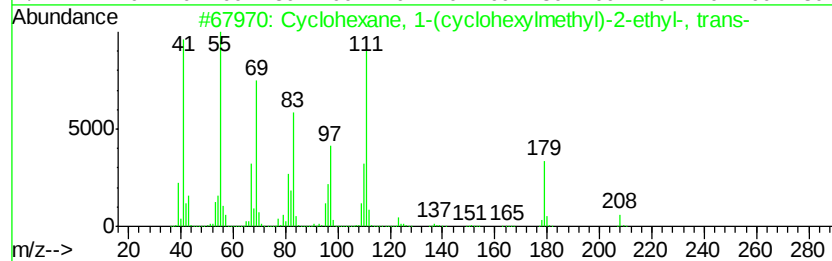
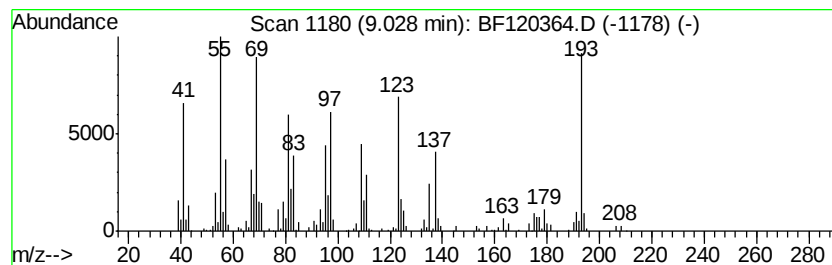
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Peak Number 3 unknown9.03 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.03	3.22 ng	339967	Acenaphthene-d10	9.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-92-8	38
2		2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	27
3		Silane, [(11-chloroundecyl)oxy]t...	278	C14H31ClOSi	026305-82-8	27
4		1-Decene, 10-bromo-	218	C10H19Br	062871-09-4	22
5		6-Bromo-2,2-dimethylcyclohexanone	204	C8H13BrO	021690-26-6	14



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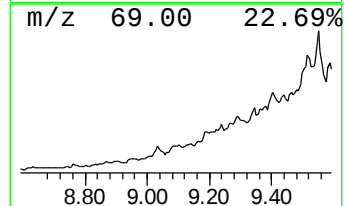
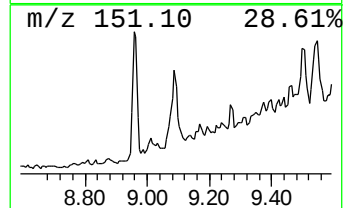
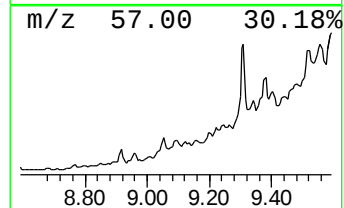
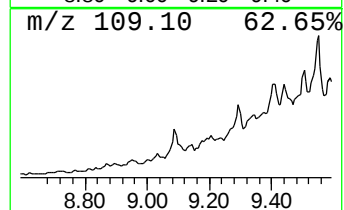
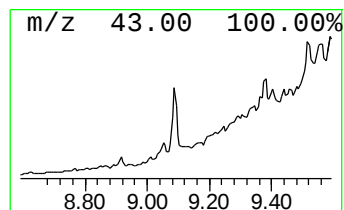
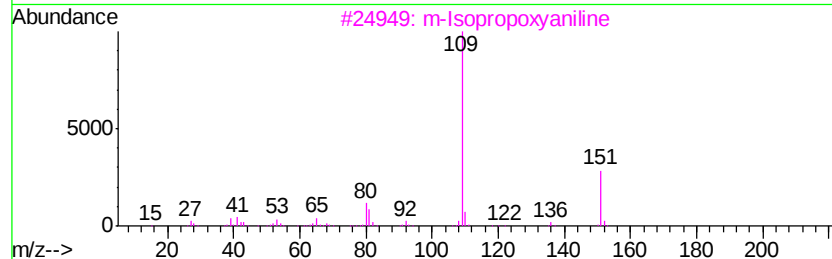
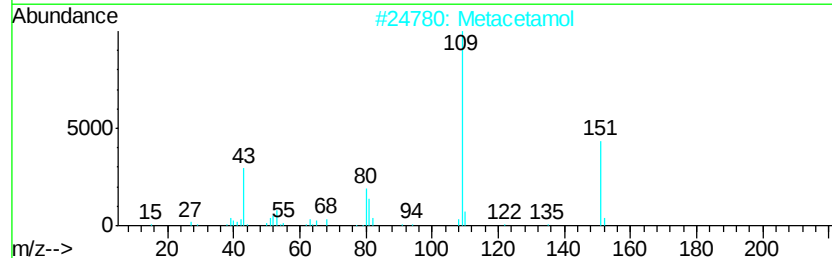
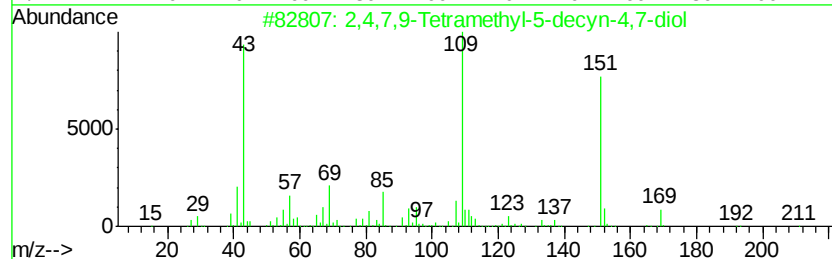
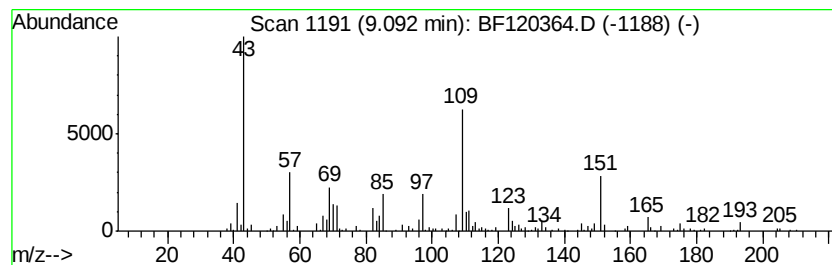
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	3.79 ng	399768	Acenaphthene-d10	9.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	72		
2	Metacetamol	151	C8H9NO2	000621-42-1	47		
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47		
4	Methyl 3-(2-formylethyl)-3-nonen...	226	C13H22O3	094608-90-9	45		
5	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	42		



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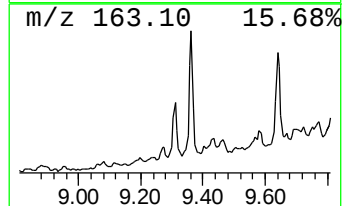
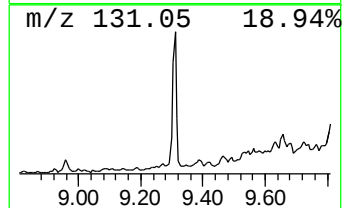
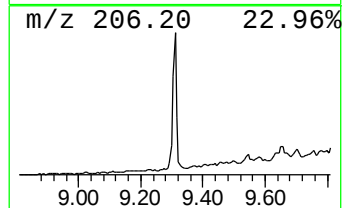
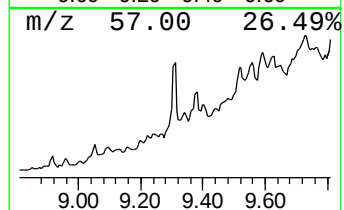
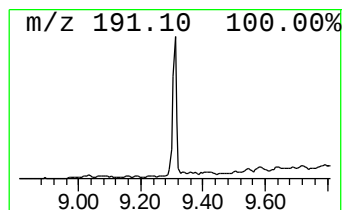
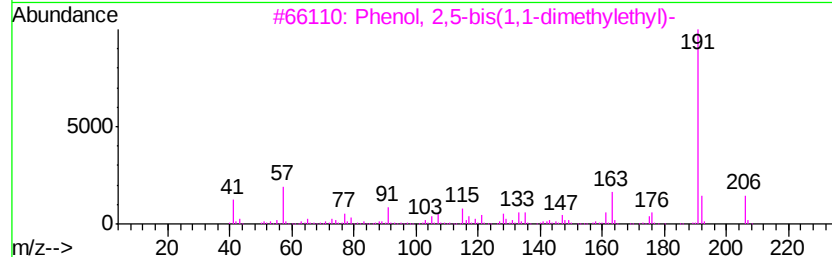
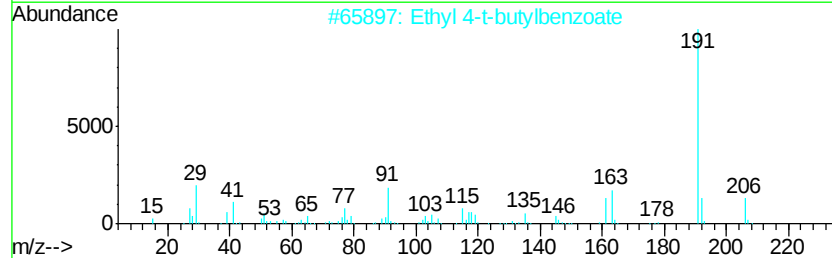
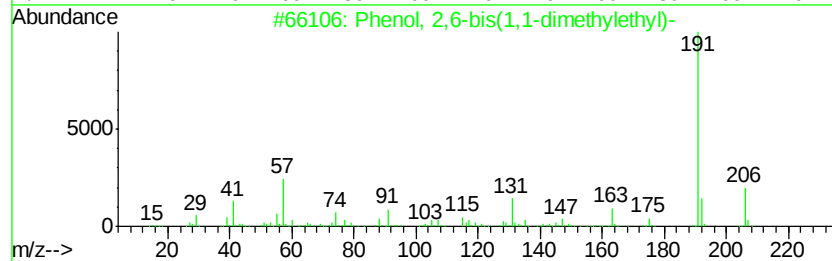
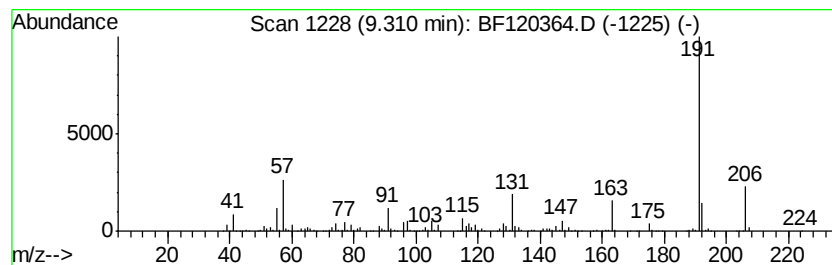
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Peak Number 5 Phenol, 2,6-bis(1,1-dimethylethyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.31	8.63 ng	910846	Acenaphthene-d10		9.64	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol,	2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2	Ethyl 4-t-butylbenzoate		206	C13H18O2	005406-57-5	74
3	Phenol,	2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	72
4	Phenol,	2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	72
5	4'-Diethylaminoacetanilide		206	C12H18N2O	005326-57-8	64



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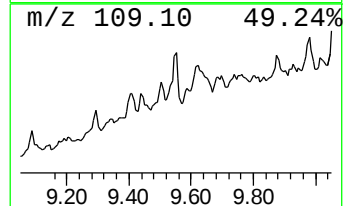
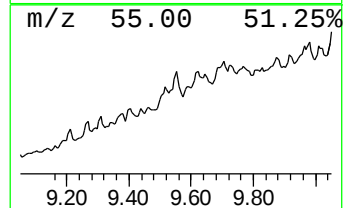
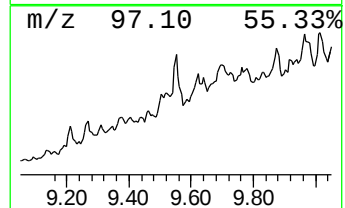
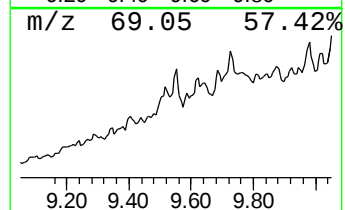
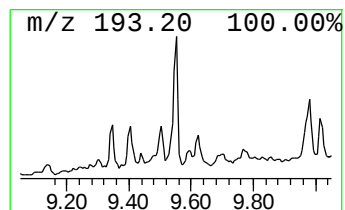
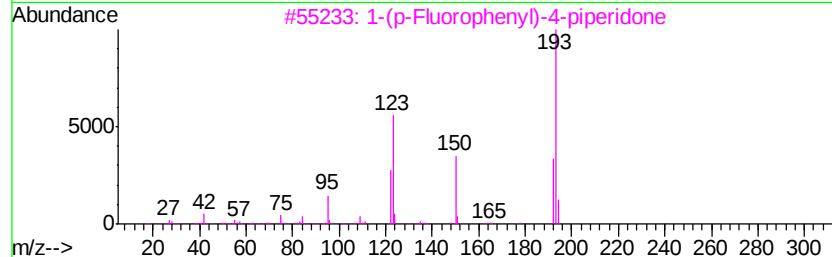
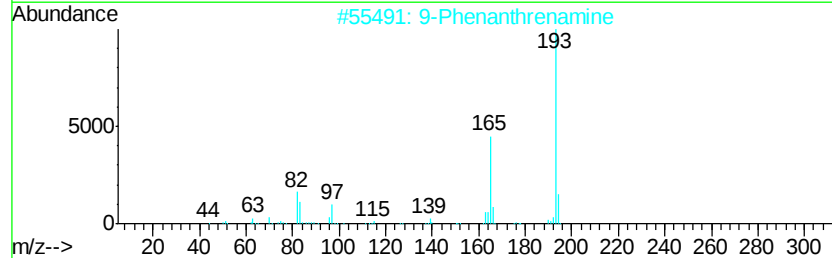
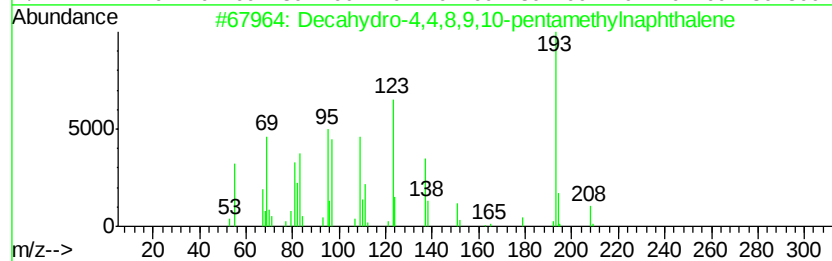
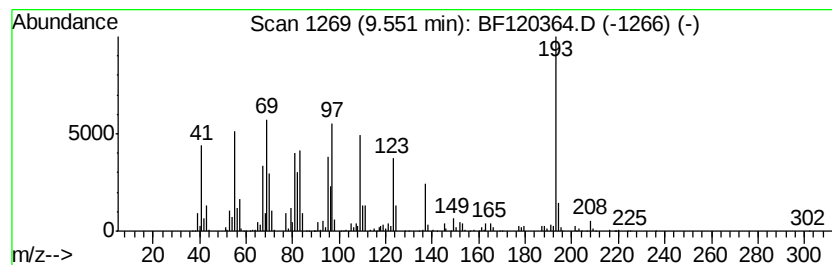
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Peak Number 6 Decahydro-4,4,8,9,10-pentam... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	17.00 ng	1794470	Acenaphthene-d10	9.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	60
2		9-Phenanthrenamine	193	C14H11N	000947-73-9	38
3		1-(p-Fluorophenyl)-4-piperidone	193	C11H12FN0	1000238-56-7	35
4		Butan-2-one, 1-[3-(3,3-dimethyl-...	278	C16H26N2O2	1000303-34-2	22
5		1-Anthracenamine	193	C14H11N	000610-49-1	22



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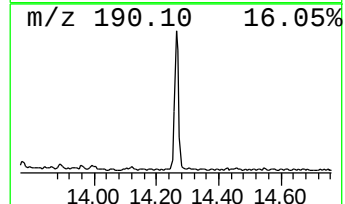
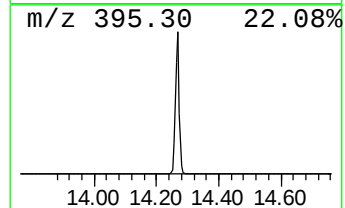
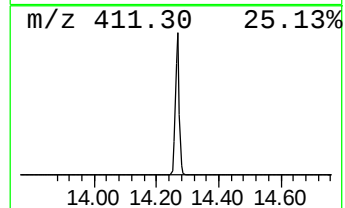
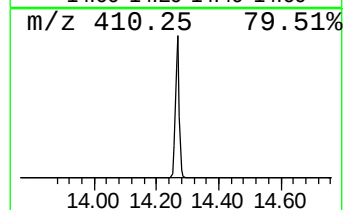
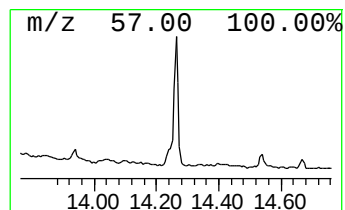
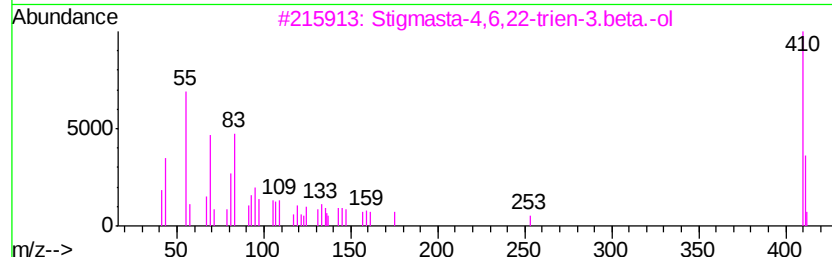
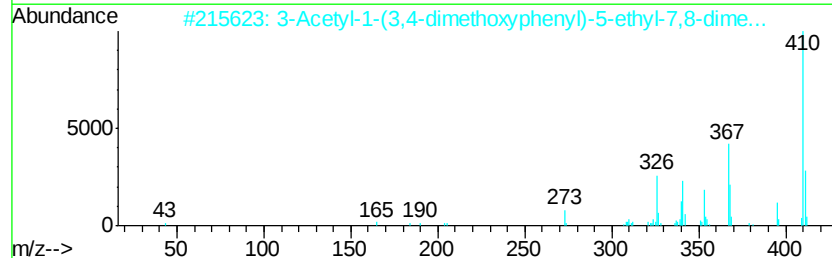
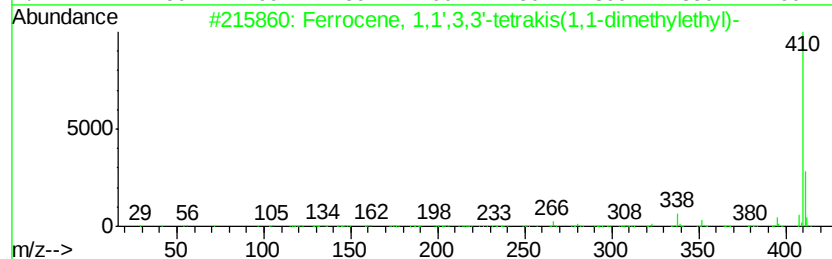
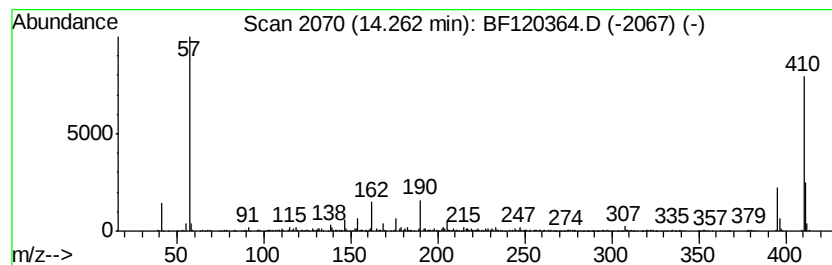
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Ferrocene, 1,1',3,3'-tetrak... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.26	12.27 ng	1371230	Chrysene-d12	13.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	53
2		3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	50
3		Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	43
4		9-Chloro-4,5-dihydro-4-[3,4,5-tr...	410	C22H19ClN2O4	1000212-48-1	40
5		6,9-Methanobenzo[h]pentaphene-5,...	410	C27H22O4	057427-50-6	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051920\
Data File : BF120364.D
Acq On : 19 May 2020 15:21
Operator : MA/SJ
Sample : L2686-02 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

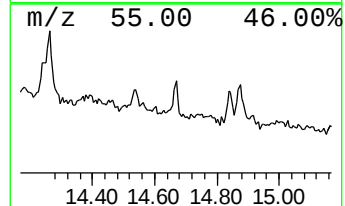
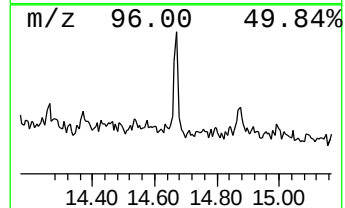
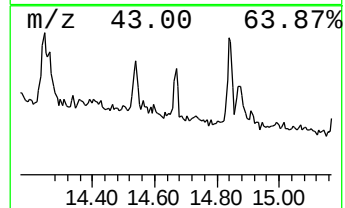
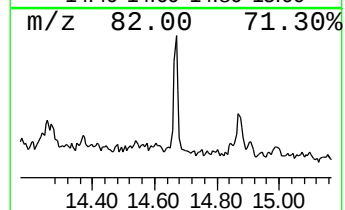
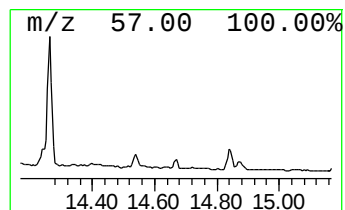
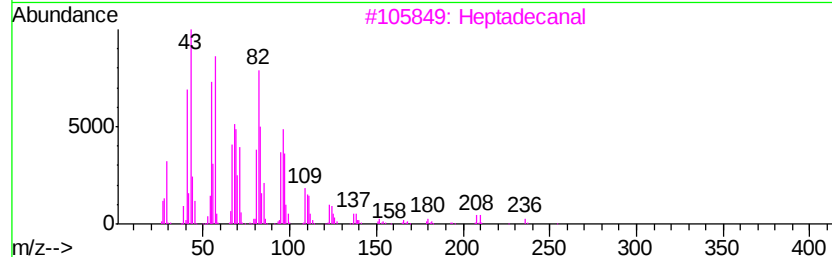
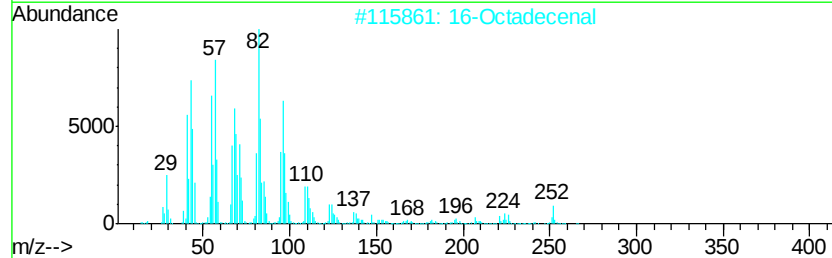
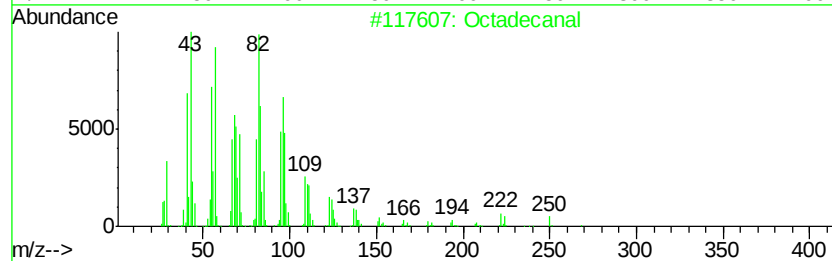
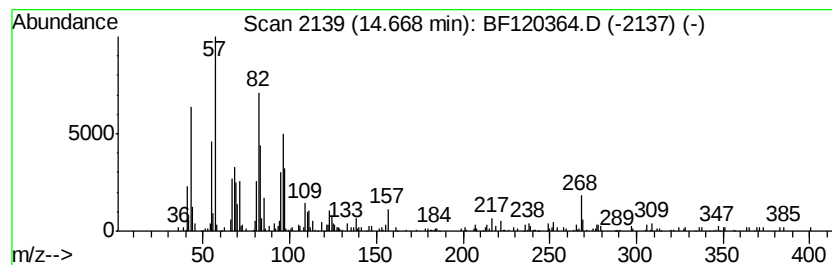
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	3.29 ng	234123	Perylene-d12	15.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal		268	C18H36O	000638-66-4	83
2	16-Octadecenal		266	C18H34O	056554-87-1	72
3	Heptadecanal		254	C17H34O	1000376-70-0	62
4	17-Octadecenal		266	C18H34O	056554-86-0	62
5	7-Azabicyclo[4.1.0]heptane, 1-me...		111	C7H13N	025022-25-7	58



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051920\
Data File : BF120364.D
Acq On : 19 May 2020 15:21
Operator : MA/SJ
Sample : L2686-02 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

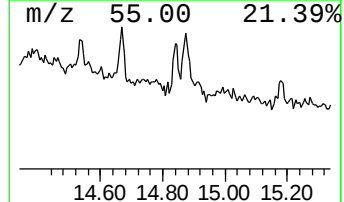
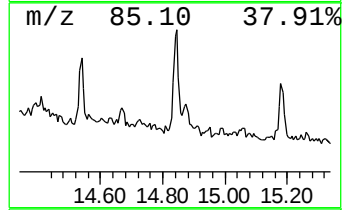
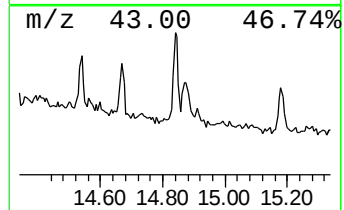
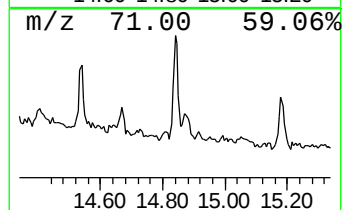
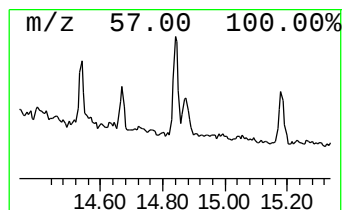
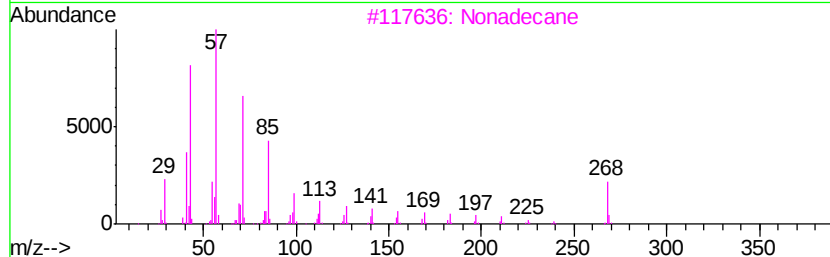
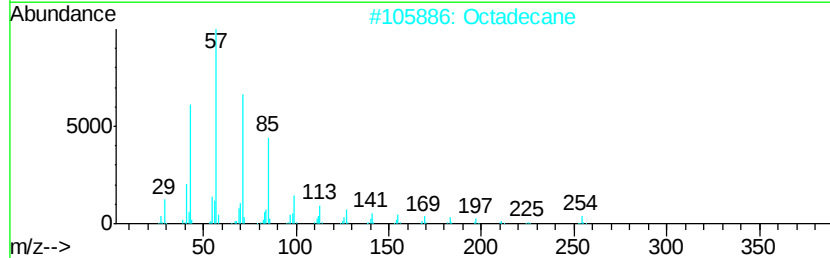
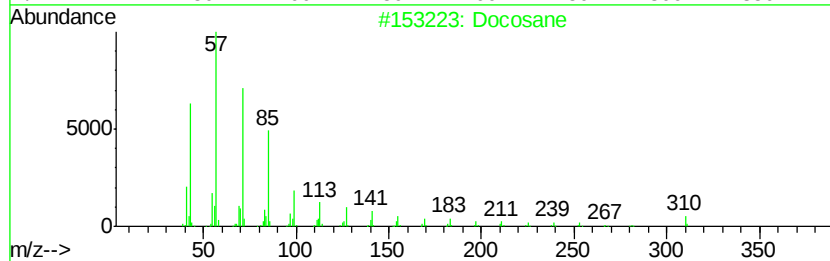
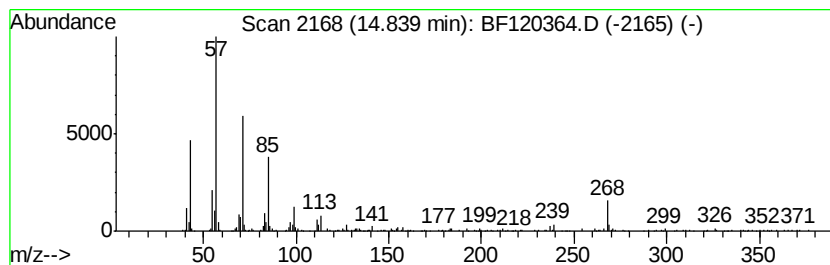
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	4.19 ng	298520	Perylene-d12	15.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane		310	C22H46	000629-97-0	95
2	Octadecane		254	C18H38	000593-45-3	94
3	Nonadecane		268	C19H40	000629-92-5	74
4	Heptacosane		380	C27H56	000593-49-7	68
5	Tridecane		184	C13H28	000629-50-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051920\
Data File : BF120364.D
Acq On : 19 May 2020 15:21
Operator : MA/SJ
Sample : L2686-02 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-214

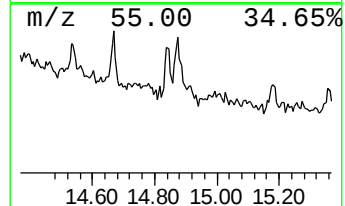
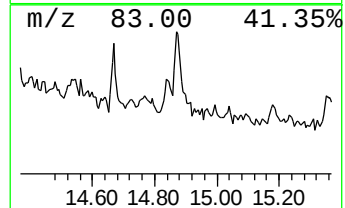
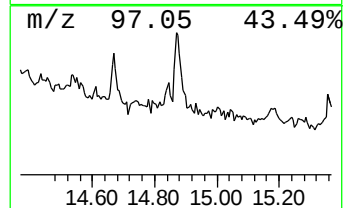
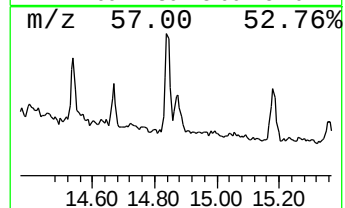
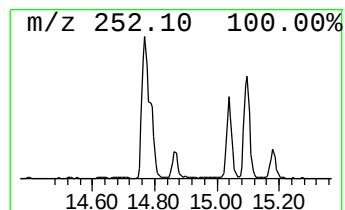
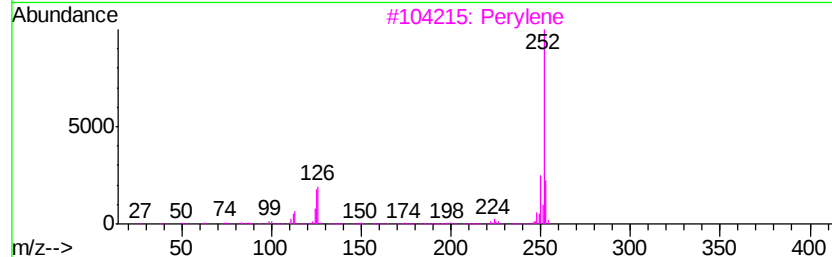
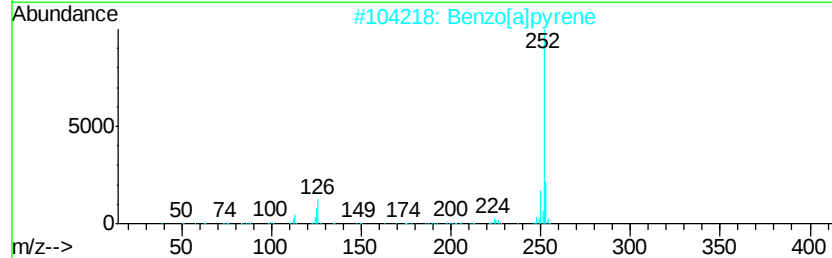
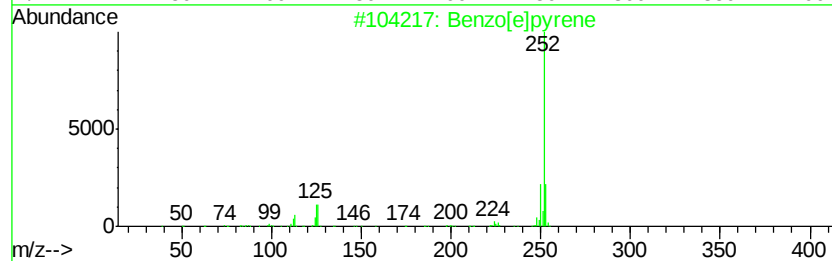
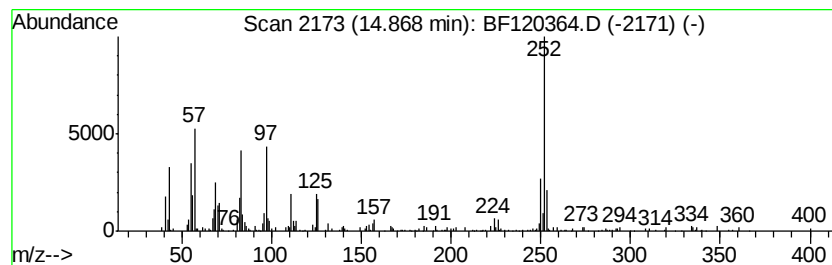
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.38 ng	311873	Perylene-d12	15.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	70
2		Benzo[a]pyrene	252	C20H12	000050-32-8	49
3		Perylene	252	C20H12	000198-55-0	49
4		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	45
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF051920\
Data File : BF120364.D
Acq On : 19 May 2020 15:21
Operator : MA/SJ
Sample : L2686-02 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051420.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
Trisulfide, bis(1...	8.58	2.5	ng	234821	2	7.88	1902360	20.0
unknown9.03	9.03	3.2	ng	339967	3	9.64	2111190	20.0
2,4,7,9-Tetrameth...	9.09	3.8	ng	399768	3	9.64	2111190	20.0
Phenol, 2,6-bis(1...	9.31	8.6	ng	910846	3	9.64	2111190	20.0
Decahydro-4,4,8,9...	9.55	17.0	ng	1794470	3	9.64	2111190	20.0
Ferrocene, 1,1',3...	14.26	12.3	ng	1371230	5	13.77	2234730	20.0
Octadecanal	14.67	3.3	ng	234123	6	15.15	1423310	20.0
Docosane	14.84	4.2	ng	298520	6	15.15	1423310	20.0
Benzo[e]pyrene	14.87	4.4	ng	311873	6	15.15	1423310	20.0