

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
 Data File : BF126282.D
 Acq On : 20 Dec 2021 17:13
 Operator : JU/CG
 Sample : M5122-02
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 369

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126282.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	600758	633189	15.80%	1.887%
2	2.222	18	23	29	rVB	89348	116903	2.92%	0.348%
3	4.404	389	394	400	rBV	38080	43536	1.09%	0.130%
4	5.028	495	500	512	rVB	1214254	1599882	39.93%	4.767%
5	5.434	564	569	572	rBV	3889753	4006784	100.00%	11.939%
6	5.834	633	637	643	rBV	200102	171220	4.27%	0.510%
7	6.445	735	741	744	rBV	3483812	3809457	95.08%	11.351%
8	6.816	800	804	807	rBV	1173246	896834	22.38%	2.672%
9	7.375	894	899	902	rBV	2444327	2505029	62.52%	7.464%
10	8.098	1018	1022	1025	rBV	1327799	1118915	27.93%	3.334%
11	9.175	1200	1205	1208	rBV	3489000	3207502	80.05%	9.557%
12	9.263	1217	1220	1226	rVB2	63635	68296	1.70%	0.203%
13	9.851	1316	1320	1324	rBV	1082658	948826	23.68%	2.827%
14	9.880	1324	1325	1332	rVB	49794	42062	1.05%	0.125%
15	10.639	1450	1454	1465	rBV	1725022	1679317	41.91%	5.004%
16	11.333	1569	1572	1575	rBV	974595	877903	21.91%	2.616%
17	11.357	1575	1576	1579	rVV	286445	181478	4.53%	0.541%
18	11.410	1582	1585	1589	rVB	62735	56726	1.42%	0.169%
19	11.869	1660	1663	1666	rBV	136474	136336	3.40%	0.406%
20	11.945	1673	1676	1683	rVB	54234	81108	2.02%	0.242%
21	12.151	1709	1711	1718	rVB2	43057	47130	1.18%	0.140%
22	12.386	1745	1751	1754	rBV5	32362	41324	1.03%	0.123%
23	12.439	1754	1760	1762	rBV4	37456	50865	1.27%	0.152%
24	12.545	1775	1778	1781	rBV	612219	500870	12.50%	1.492%
25	12.774	1811	1817	1820	rBV	538623	545245	13.61%	1.625%
26	12.921	1838	1842	1846	rBV	2882260	2695788	67.28%	8.032%
27	13.080	1862	1869	1870	rBV5	35777	51633	1.29%	0.154%
28	13.104	1870	1873	1875	rVB	67960	62821	1.57%	0.187%
29	13.168	1880	1884	1886	rBV2	59599	57346	1.43%	0.171%
30	13.204	1886	1890	1893	rBV	57699	65138	1.63%	0.194%
31	13.357	1913	1916	1919	rBV2	47496	50310	1.26%	0.150%
32	13.392	1919	1922	1929	rVB7	42288	69915	1.74%	0.208%
33	13.604	1955	1958	1964	rVB	37056	54002	1.35%	0.161%
34	13.721	1973	1978	1980	rBV2	55885	79179	1.98%	0.236%
35	13.768	1984	1986	1991	rVB2	39037	58243	1.45%	0.174%
36	13.880	2000	2005	2013	rBV4	154442	439654	10.97%	1.310%

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37	13.962	2015	2019	2023	rVV2	2144709	2485049	62.02%	7.404%
38	13.992	2023	2024	2031	rVB	290825	270789	6.76%	0.807%
39	14.068	2032	2037	2047	rBV	611589	676235	16.88%	2.015%
40	14.357	2082	2086	2090	rBV2	48740	57190	1.43%	0.170%
41	14.392	2090	2092	2096	rVB2	50509	45040	1.12%	0.134%
42	14.451	2099	2102	2105	rBV2	63983	63597	1.59%	0.189%
43	14.551	2114	2119	2125	rVB6	43936	111301	2.78%	0.332%
44	14.609	2126	2129	2133	rVB2	46762	47816	1.19%	0.142%
45	14.657	2134	2137	2140	rBV4	37750	40536	1.01%	0.121%
46	14.833	2163	2167	2173	rBV3	111111	147948	3.69%	0.441%
47	14.998	2191	2195	2198	rBV	362572	512768	12.80%	1.528%
48	15.098	2208	2212	2217	rVB3	82981	133493	3.33%	0.398%
49	15.298	2242	2246	2251	rVB	213656	267875	6.69%	0.798%
50	15.357	2251	2256	2259	rBV	242660	286161	7.14%	0.853%
51	15.421	2262	2267	2270	rBV	766186	932628	23.28%	2.779%
52	15.898	2344	2348	2353	rBV	58841	82314	2.05%	0.245%
53	16.839	2504	2508	2518	rVB2	85006	169486	4.23%	0.505%
54	16.974	2527	2531	2537	rBV4	22066	48230	1.20%	0.144%
55	17.268	2576	2581	2587	rBV2	66871	132617	3.31%	0.395%

Sum of corrected areas: 33561839

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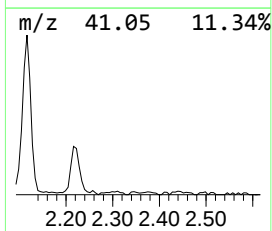
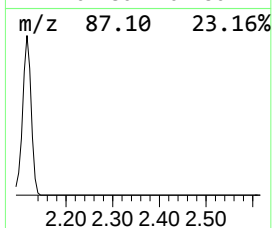
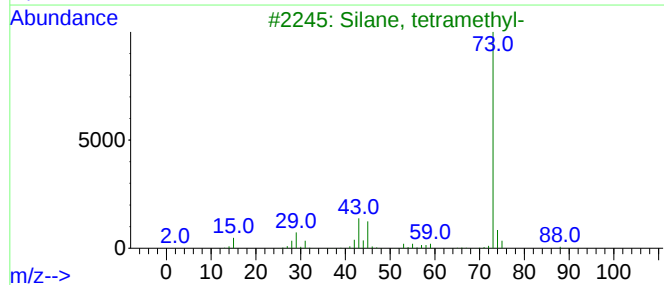
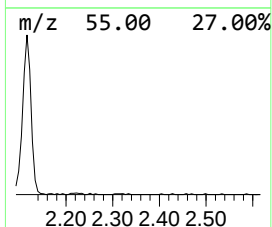
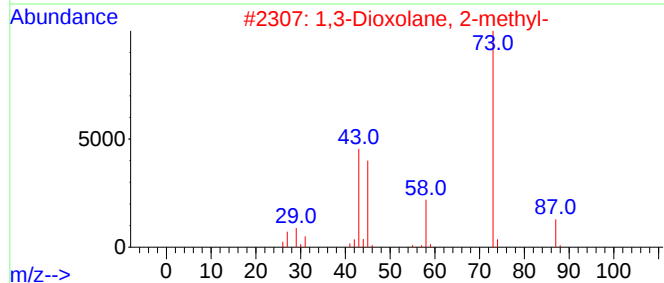
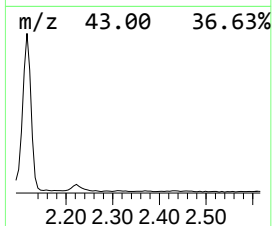
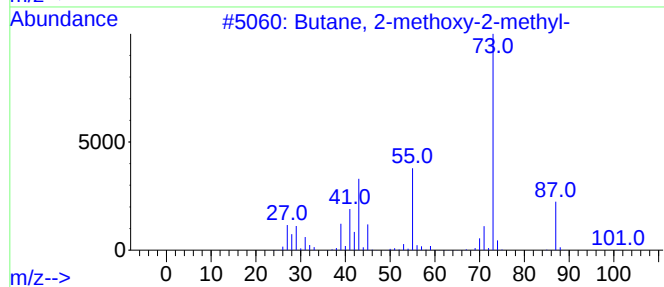
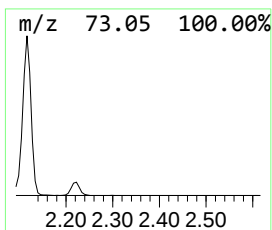
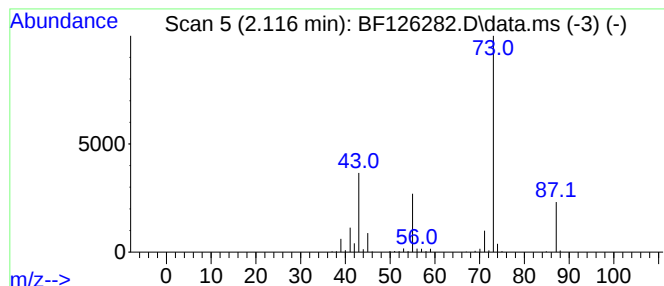
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	14.12 ng	633189	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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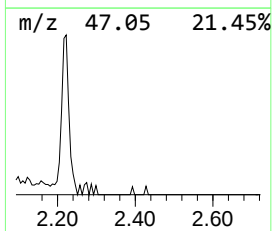
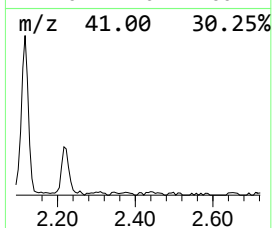
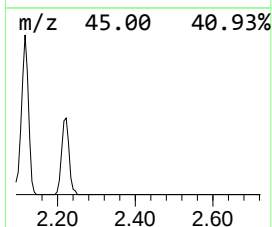
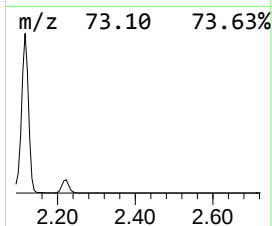
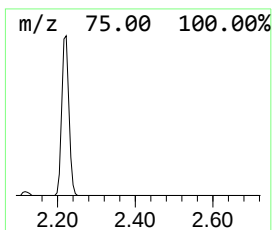
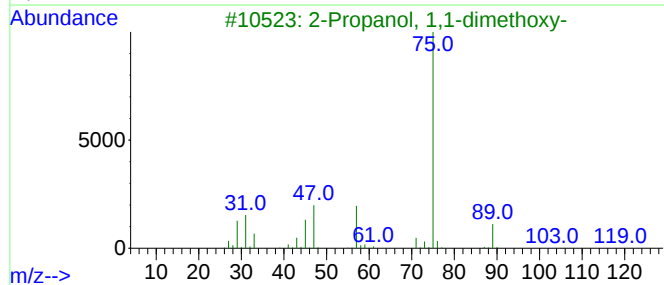
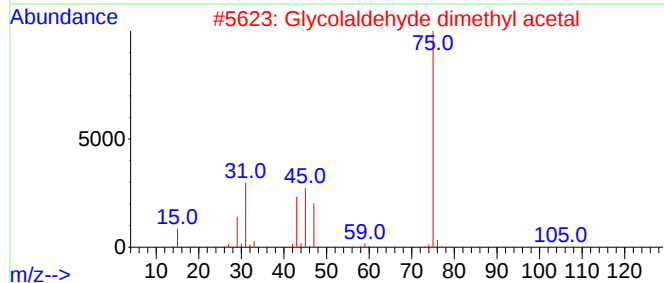
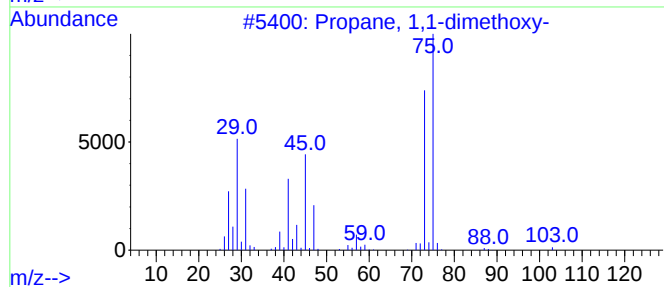
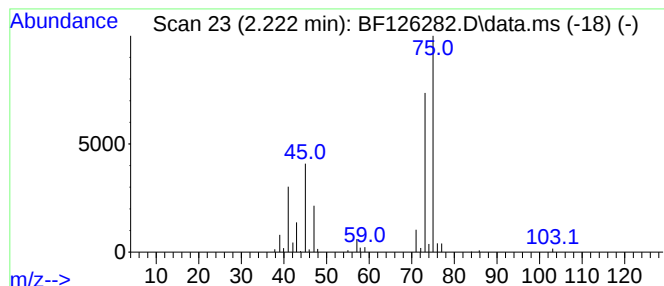
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	2.61 ng	116903	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2			Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	45
3			2-Propanol, 1,1-dimethoxy-	120	C5H12O3	042919-42-6	33
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
5			2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	10



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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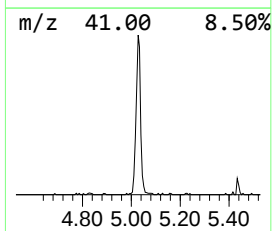
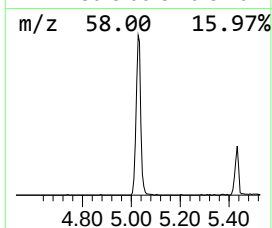
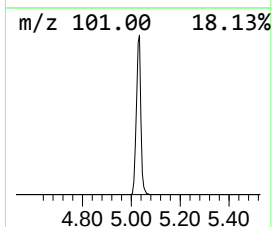
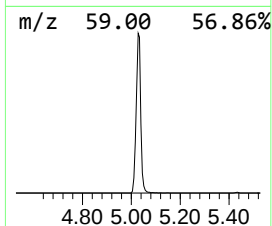
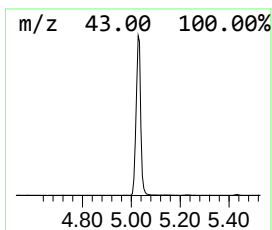
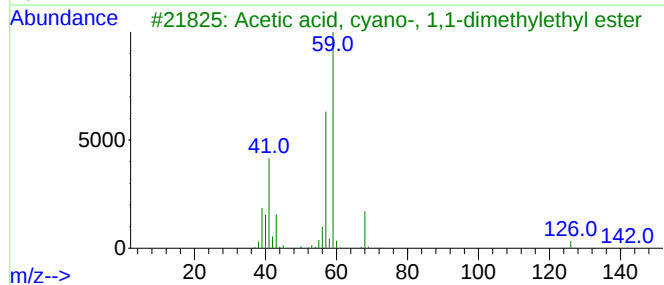
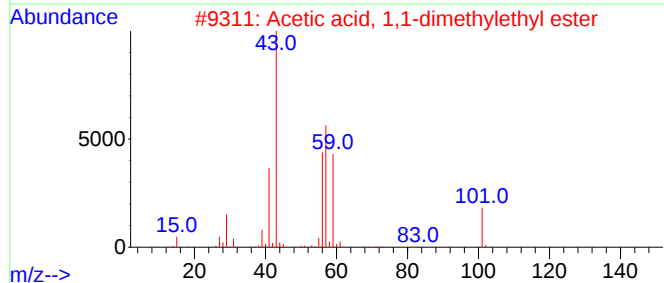
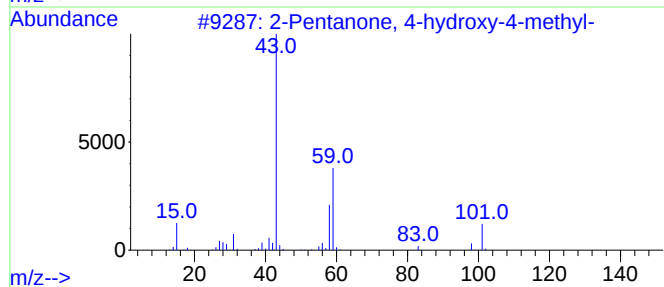
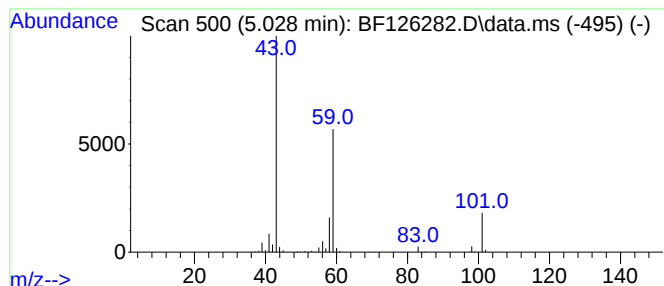
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	35.68 ng	1599880	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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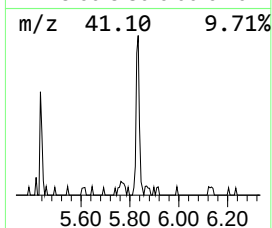
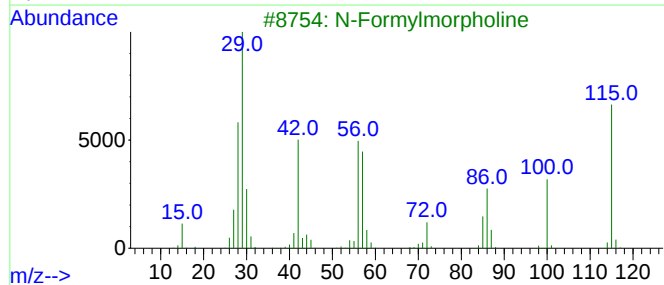
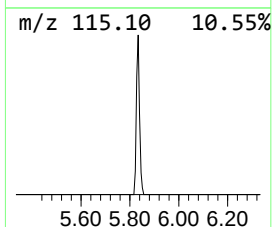
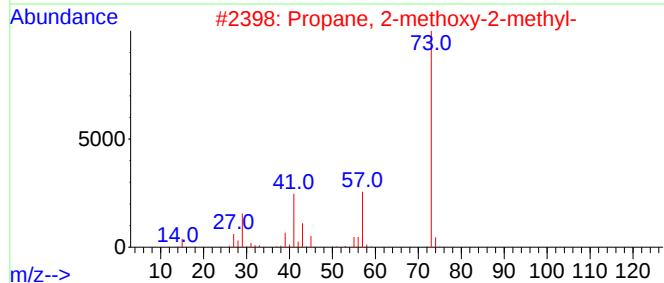
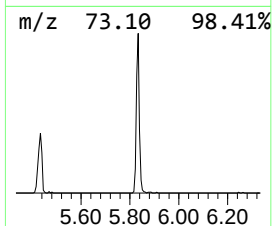
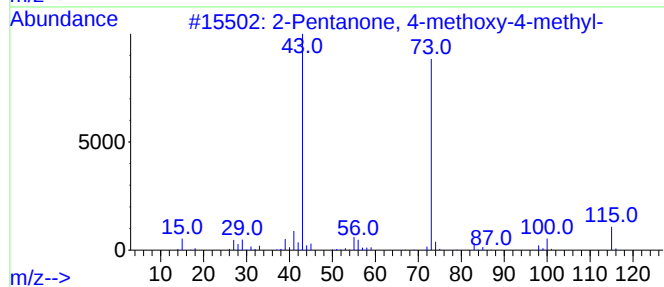
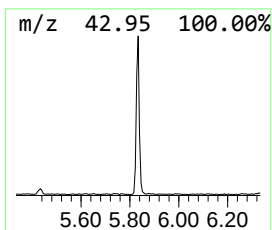
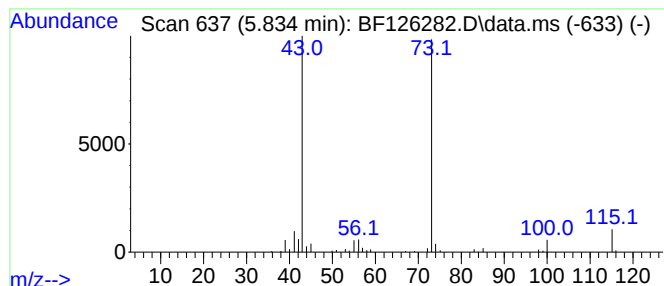
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.834	3.82 ng	171220	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
3			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
5			Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9



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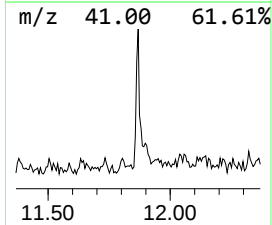
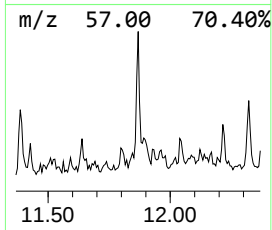
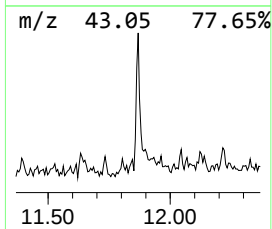
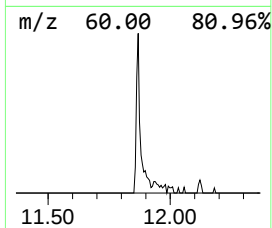
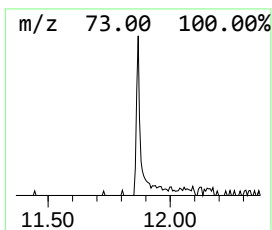
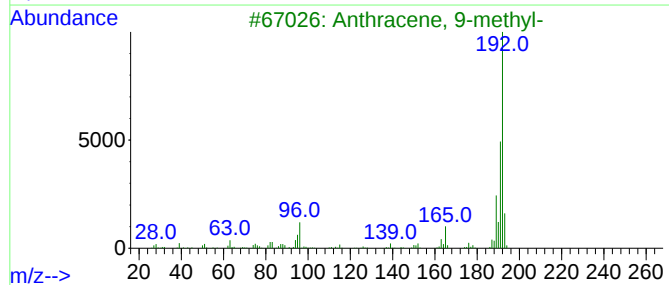
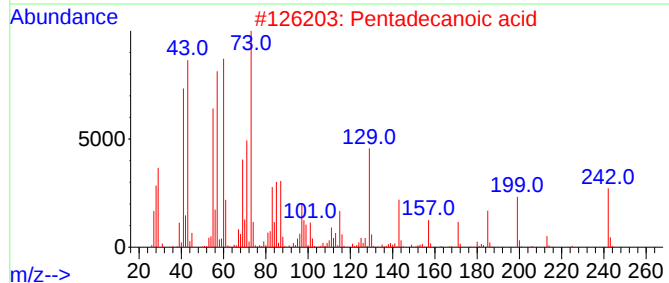
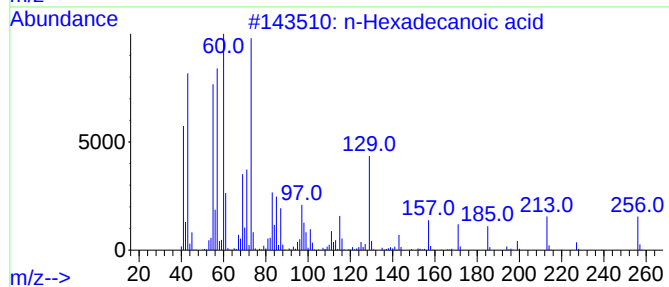
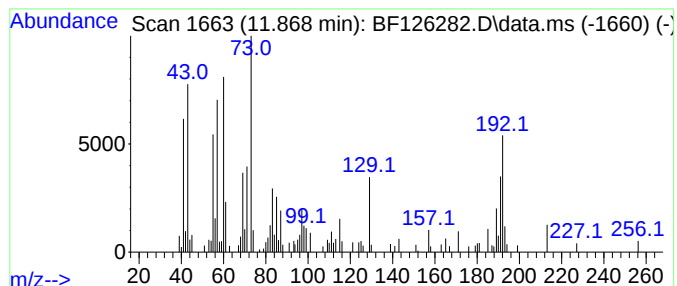
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.868	3.11 ng	136336	Phenanthrene-d10	11.333	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	56
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	25
5	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
Operator : JU/CG
Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

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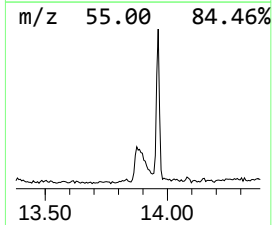
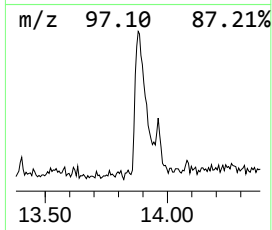
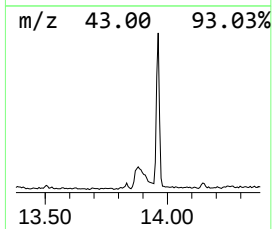
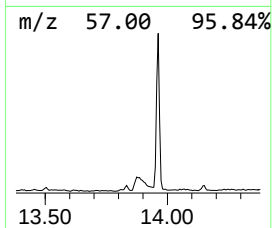
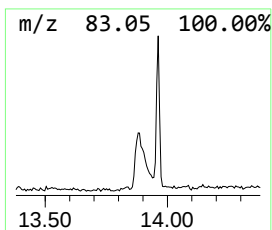
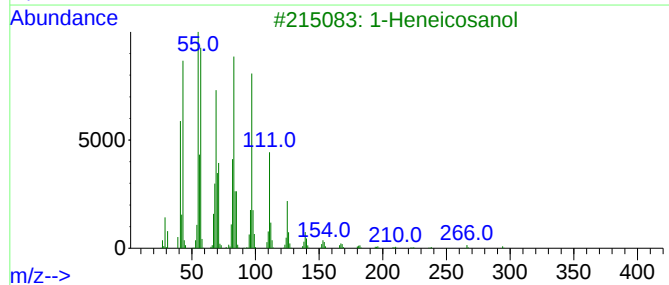
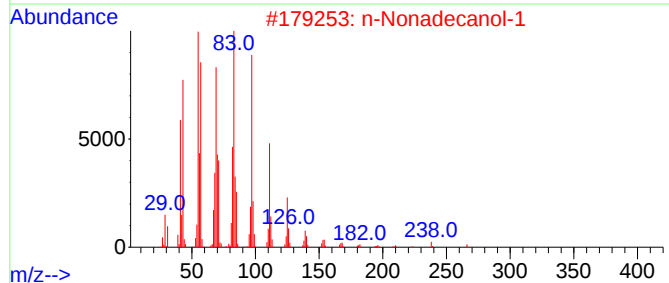
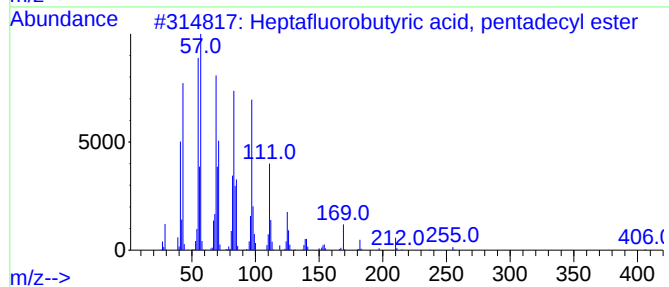
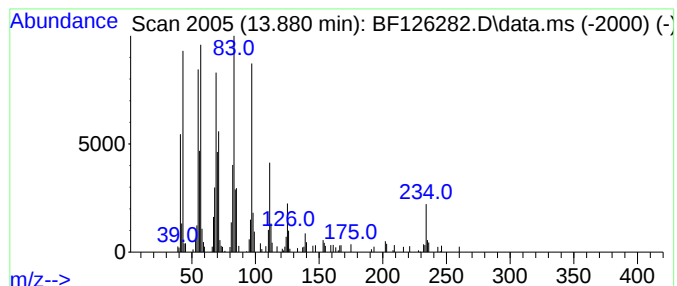
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	3.54 ng	439654	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
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Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

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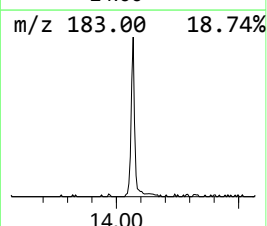
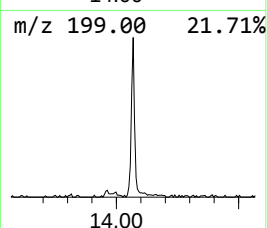
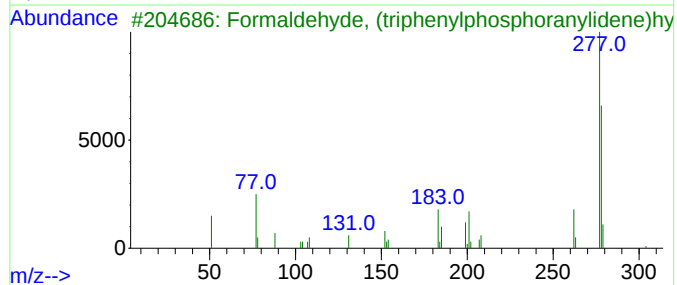
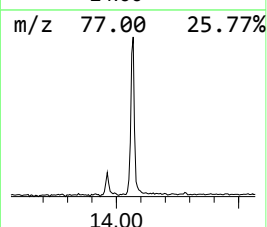
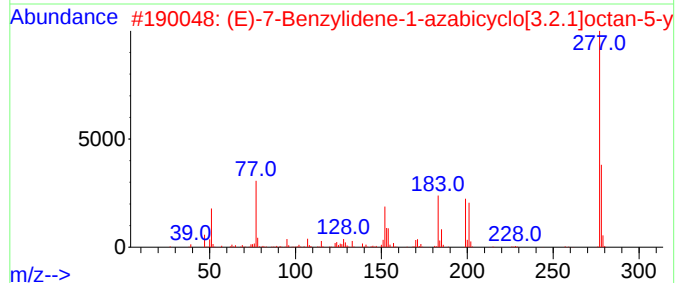
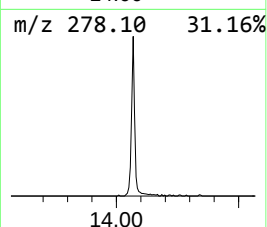
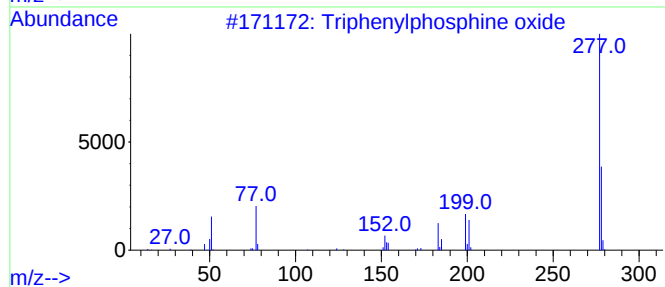
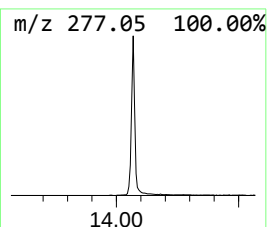
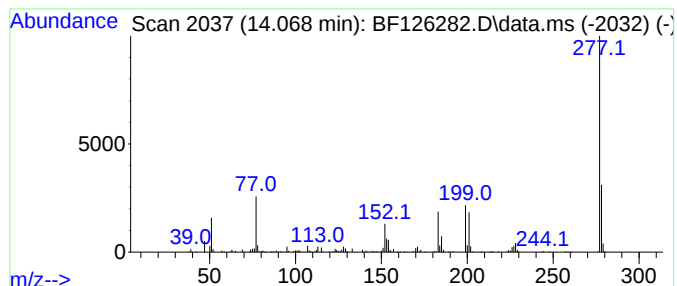
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Triphenylphosphine oxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	5.44 ng	676235	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	70
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	59
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	40
5			2-Phenyl-6-(trifluoromethyl)-1H-...	277	C15H10F3NO	1000387-59-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
Operator : JU/CG
Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

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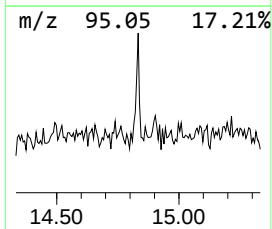
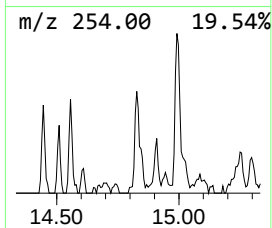
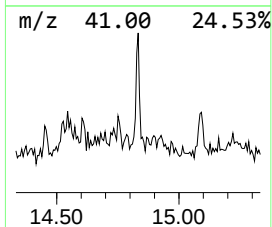
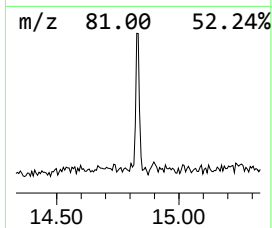
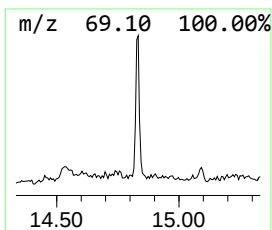
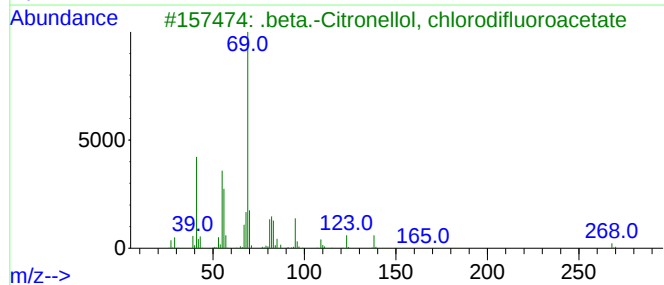
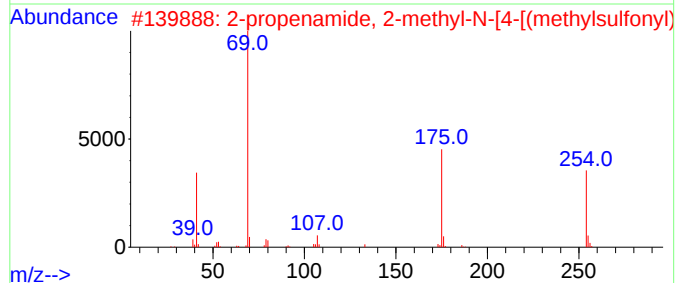
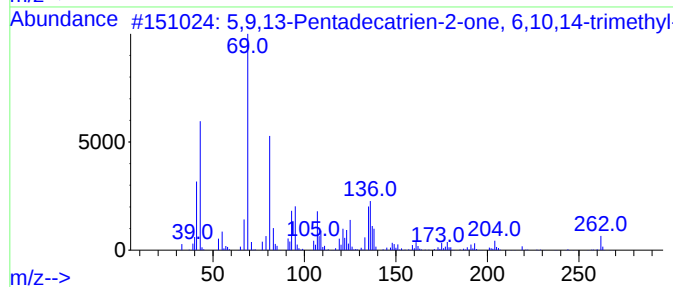
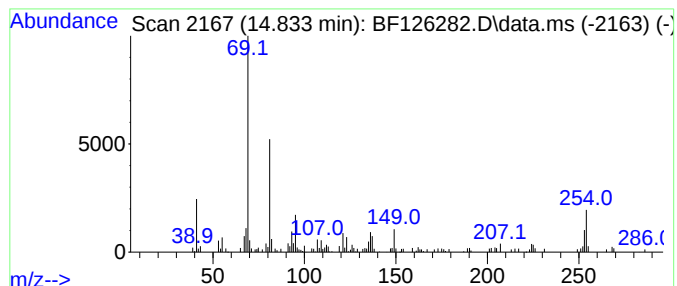
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 5,9,13-Pentadecatrien-2-one... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	3.17 ng	147948	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	000762-29-8	50		
2	2-propenamide, 2-methyl-N-[4-(m...	254	C11H14N2O3S	1000401-43-5	50		
3	.beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	49		
4	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	49		
5	Furan, 3-(4,8-dimethyl-3,7-nonad...	218	C15H22O	023262-34-2	47		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
Operator : JU/CG
Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

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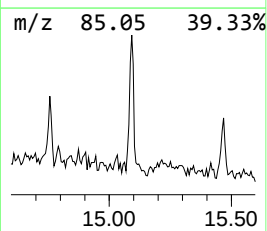
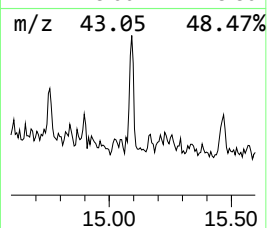
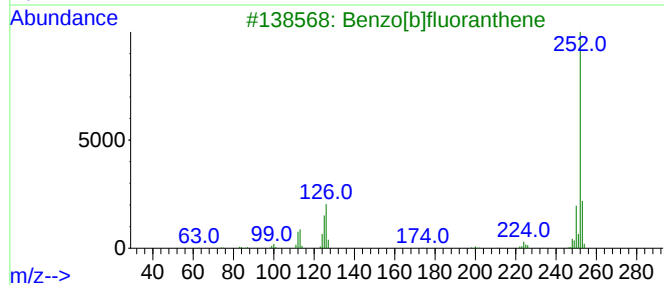
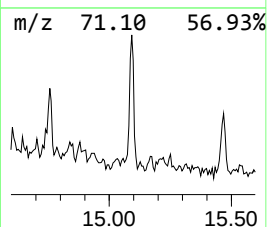
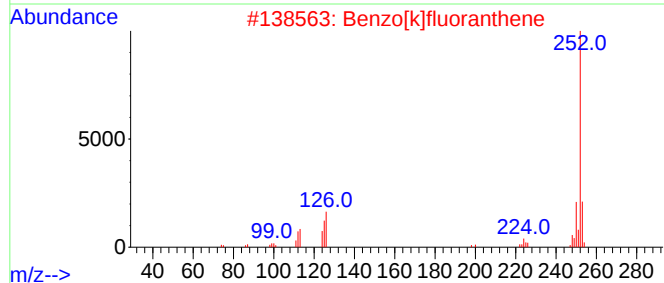
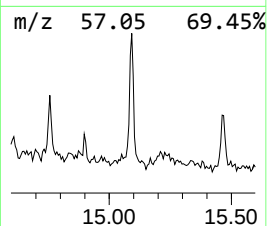
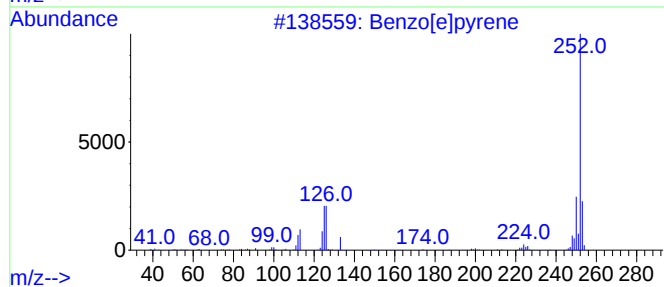
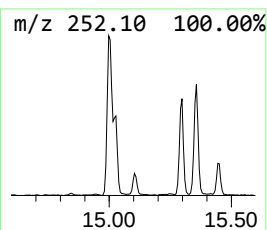
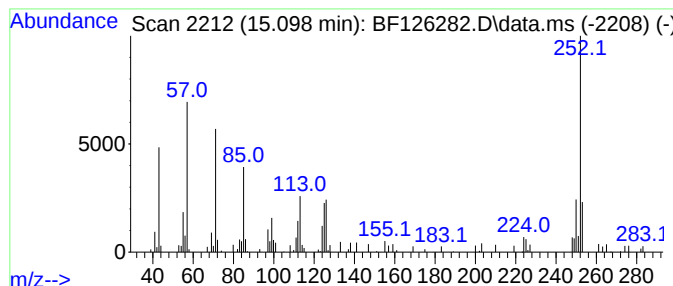
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.098	2.86 ng	133493	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	90
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	83
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	60
4			Benzo[a]pyrene	252	C20H12	000050-32-8	60
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
Operator : JU/CG
Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

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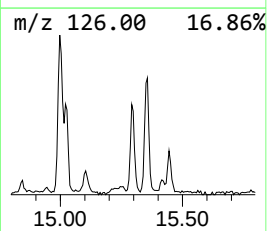
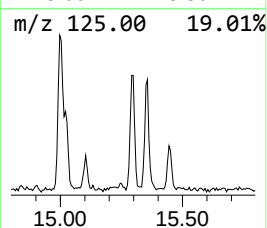
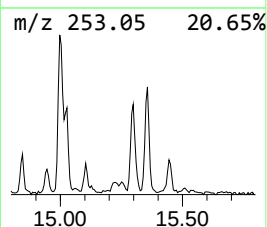
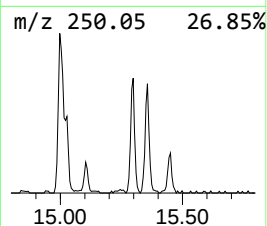
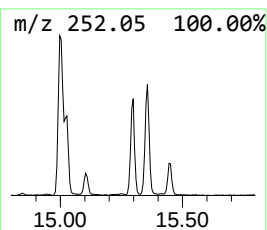
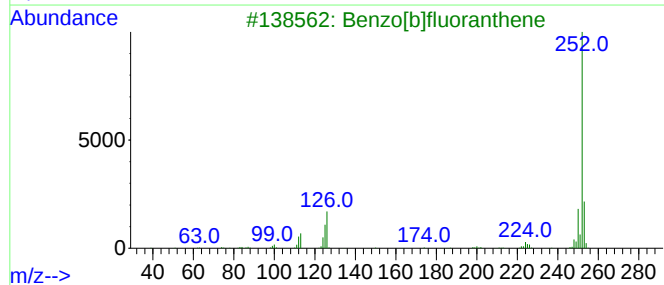
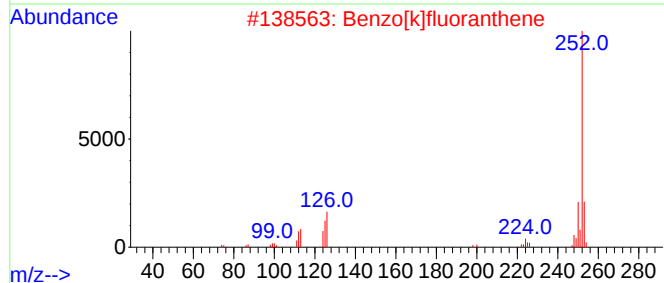
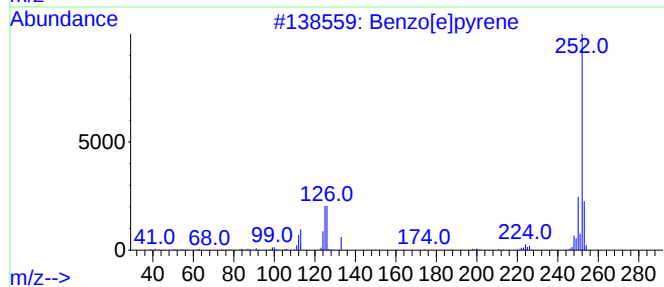
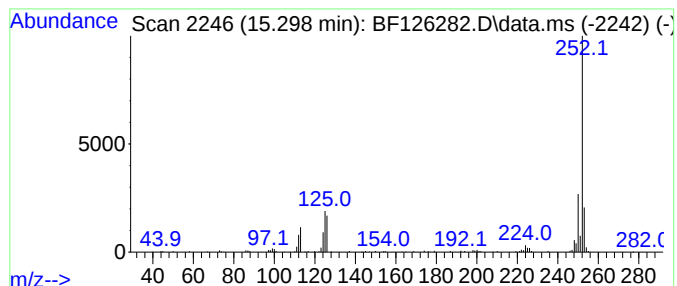
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Benzo[j]fluoranthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	5.74 ng	267875	Perylene-d12	15.421

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	98
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	97
5			Benzo[a]pyrene	252	C20H12	000050-32-8	96



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122021\
Data File : BF126282.D
Acq On : 20 Dec 2021 17:13
Operator : JU/CG
Sample : M5122-02
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Propane, 1,1-di...	2.222	2.6	ng	116903	1	6.816	896834	20.0
2-Pentanone, 4-...	5.028	35.7	ng	1599880	1	6.816	896834	20.0
2-Pentanone, 4-...	5.834	3.8	ng	171220	1	6.816	896834	20.0
n-Hexadecanoic ...	11.868	3.1	ng	136336	4	11.333	877903	20.0
Heptafluorobuty...	13.880	3.5	ng	439654	5	13.968	2485050	20.0
Triphenylphosph...	14.068	5.4	ng	676235	5	13.968	2485050	20.0
5,9,13-Pentadec...	14.833	3.2	ng	147948	6	15.421	932628	20.0
Benzo[e]pyrene	15.098	2.9	ng	133493	6	15.421	932628	20.0
Benzo[j]fluoran...	15.298	5.7	ng	267875	6	15.421	932628	20.0