

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
 Data File : BF122457.D
 Acq On : 23 Nov 2020 20:26
 Operator : JU/CG
 Sample : L4876-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TB-2D

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122457.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.151	5	11	25	rVB	426696	598809	13.61%	1.497%
2	2.257	25	29	36	rVB	53265	72922	1.66%	0.182%
3	4.457	398	403	411	rBV	128545	150770	3.43%	0.377%
4	5.087	502	510	513	rBV	2080424	2754539	62.61%	6.887%
5	5.492	573	579	582	rBV	3871996	3863338	87.81%	9.659%
6	5.875	641	644	652	rVB	274819	243361	5.53%	0.608%
7	6.498	744	750	754	rBV	3752655	4147481	94.27%	10.370%
8	6.863	808	812	815	rBV	1280365	972420	22.10%	2.431%
9	7.428	903	908	911	rBV	2598602	2477129	56.30%	6.194%
10	8.151	1027	1031	1034	rBV	1365629	1234680	28.06%	3.087%
11	9.227	1209	1214	1217	rBV	4820002	4399798	100.00%	11.001%
12	9.622	1277	1281	1290	rBV	159452	158382	3.60%	0.396%
13	9.910	1325	1330	1333	rBV	1474925	1319152	29.98%	3.298%
14	10.698	1459	1464	1475	rBV	2826716	2725712	61.95%	6.815%
15	11.398	1579	1583	1585	rBV	1339943	1234192	28.05%	3.086%
16	11.416	1585	1586	1590	rVV	206841	179149	4.07%	0.448%
17	11.468	1593	1595	1599	rVB	68497	64966	1.48%	0.162%
18	11.927	1670	1673	1678	rBV	205504	193281	4.39%	0.483%
19	12.010	1684	1687	1690	rBV	75637	84223	1.91%	0.211%
20	12.345	1739	1744	1747	rBV2	75149	71206	1.62%	0.178%
21	12.380	1747	1750	1752	rBV	55044	47530	1.08%	0.119%
22	12.610	1786	1789	1793	rBV	554339	478831	10.88%	1.197%
23	12.657	1794	1797	1802	rVB2	76325	80344	1.83%	0.201%
24	12.710	1802	1806	1812	rBV2	63078	78148	1.78%	0.195%
25	12.839	1822	1828	1831	rBV	526611	523313	11.89%	1.308%
26	12.892	1834	1837	1845	rVB3	38876	58554	1.33%	0.146%
27	12.986	1849	1853	1857	rVV	4391229	3953849	89.86%	9.886%
28	13.062	1861	1866	1869	rBV2	41294	60065	1.37%	0.150%
29	13.121	1873	1876	1879	rBV	138215	131827	3.00%	0.330%
30	13.168	1882	1884	1887	rVB2	118861	104717	2.38%	0.262%
31	13.233	1887	1895	1898	rBV	110604	139698	3.18%	0.349%
32	13.274	1898	1902	1905	rVV2	83667	88328	2.01%	0.221%
33	13.680	1968	1971	1975	rVB4	41367	57690	1.31%	0.144%
34	13.792	1986	1990	1992	rBV2	40377	50071	1.14%	0.125%
35	13.839	1996	1998	2005	rVV3	54227	79142	1.80%	0.198%
36	13.898	2005	2008	2022	rVV3	225445	445772	10.13%	1.115%

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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-BF110920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.039	2027	2032	2035	rVV2	1504791	1828068	41.55%	4.571%
38	14.062	2035	2036	2042	rVB	325570	296246	6.73%	0.741%
39	14.145	2048	2050	2053	rBV	71252	63889	1.45%	0.160%
40	14.427	2095	2098	2102	rVB	83489	73041	1.66%	0.183%
41	14.462	2102	2104	2108	rVB	55405	46674	1.06%	0.117%
42	14.521	2108	2114	2116	rBV4	94336	139000	3.16%	0.348%
43	14.574	2121	2123	2127	rVB4	68830	70576	1.60%	0.176%
44	14.909	2177	2180	2182	rBV	47838	58063	1.32%	0.145%
45	15.086	2206	2210	2213	rBV	370312	552323	12.55%	1.381%
46	15.198	2226	2229	2233	rVB	99508	106966	2.43%	0.267%
47	15.392	2258	2262	2268	rBV	242957	326534	7.42%	0.816%
48	15.456	2268	2273	2278	rVB	444290	544615	12.38%	1.362%
49	15.521	2279	2284	2288	rBV	1127929	1447937	32.91%	3.620%
50	16.086	2376	2380	2385	rBV3	49478	83413	1.90%	0.209%
51	16.821	2496	2505	2513	rBV4	38647	143865	3.27%	0.360%
52	16.992	2528	2534	2541	rVB2	184687	359009	8.16%	0.898%
53	17.168	2560	2564	2570	rVB2	40738	73325	1.67%	0.183%
54	17.239	2570	2576	2579	rBV3	45851	89404	2.03%	0.224%
55	17.439	2603	2610	2619	rBV	136289	279845	6.36%	0.700%
56	17.674	2647	2650	2655	rVB	52616	89212	2.03%	0.223%

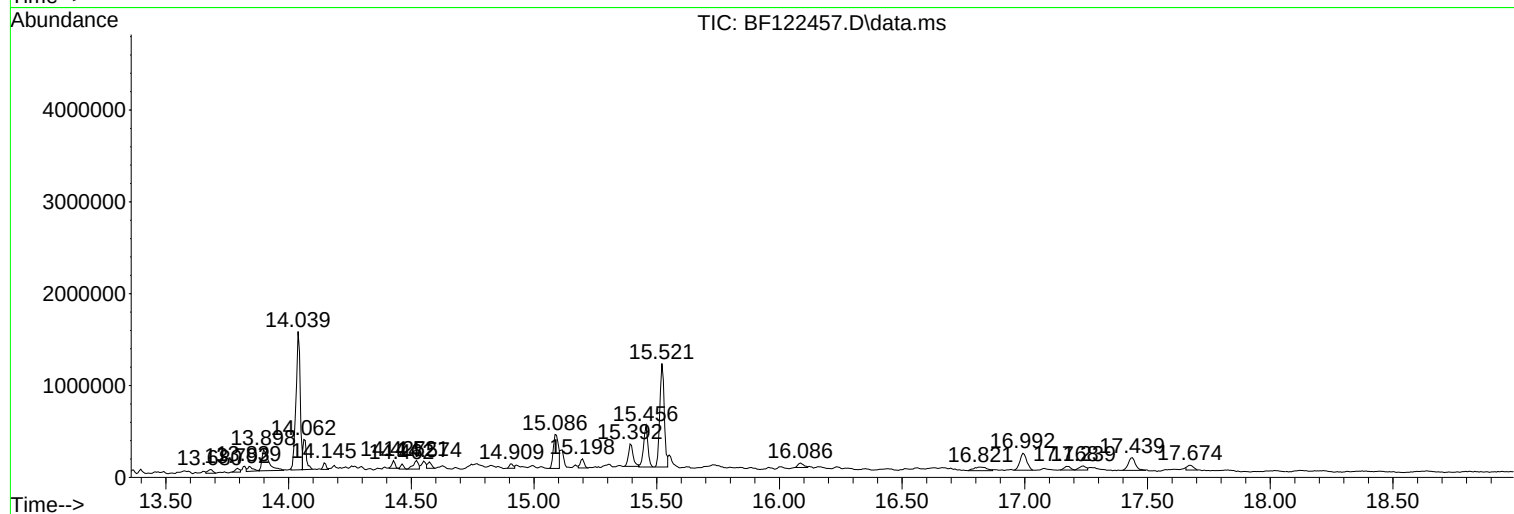
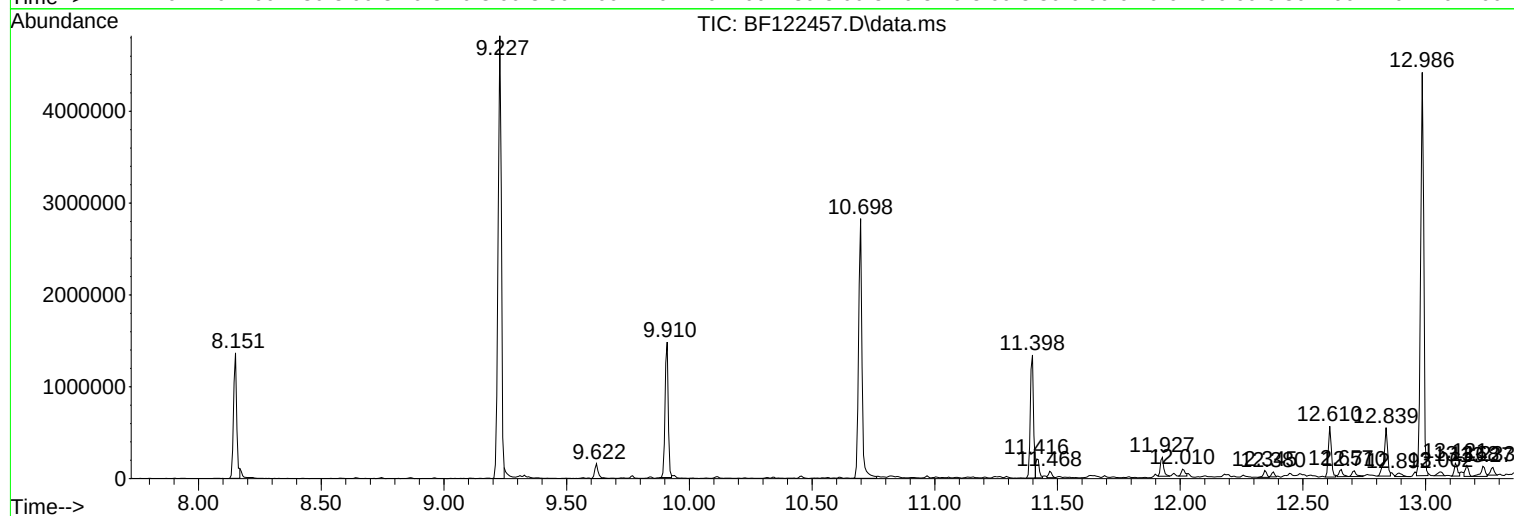
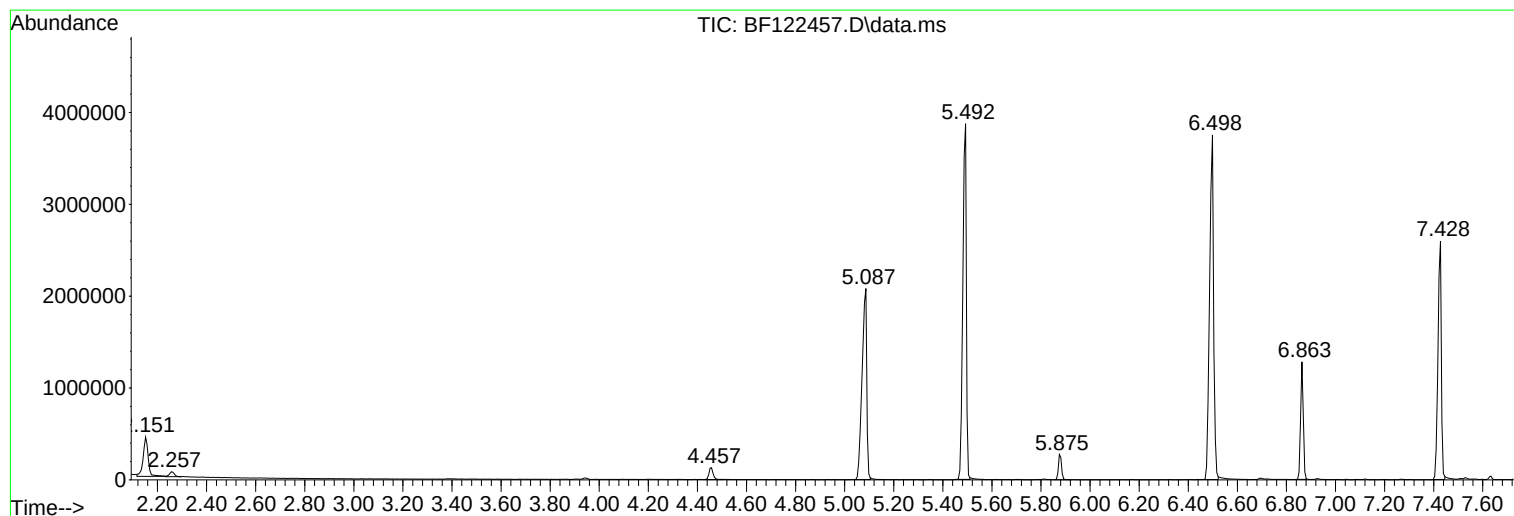
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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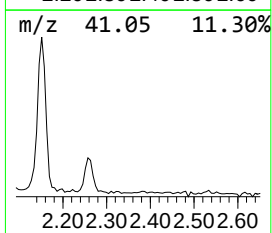
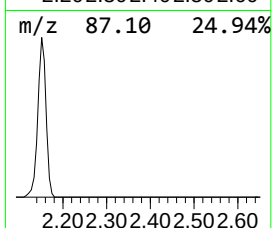
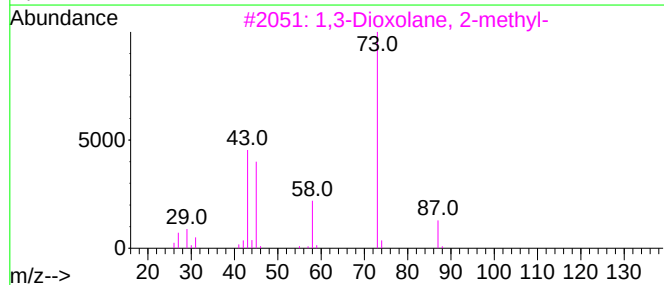
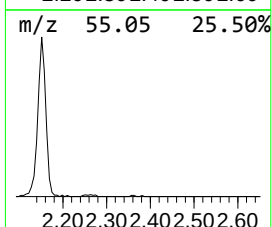
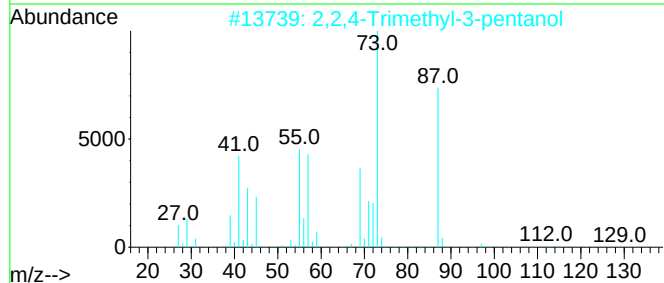
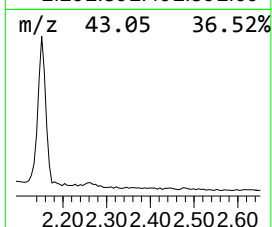
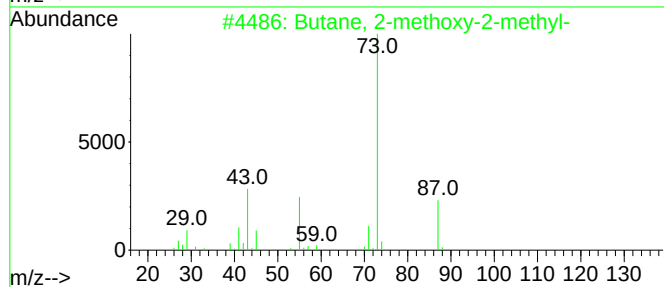
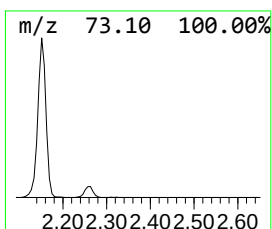
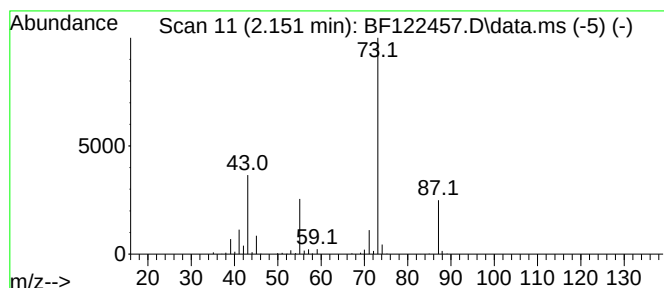
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.151	12.32 ng	598809	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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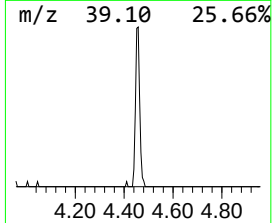
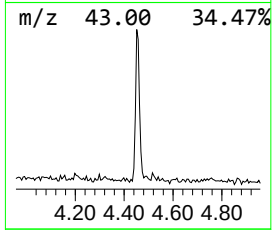
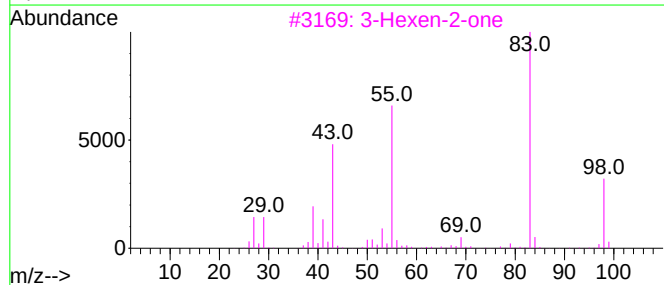
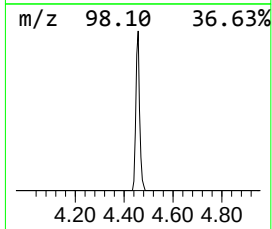
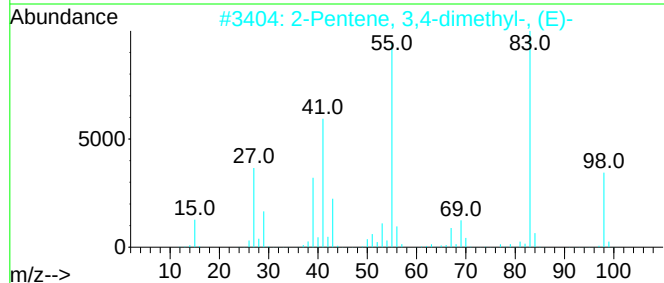
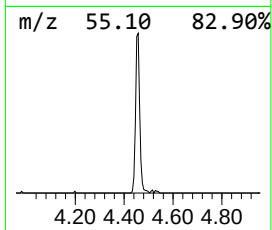
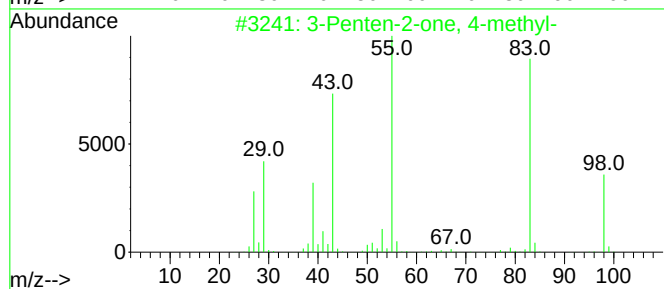
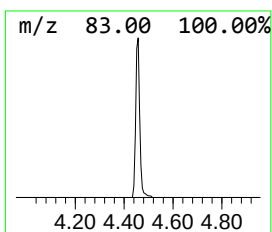
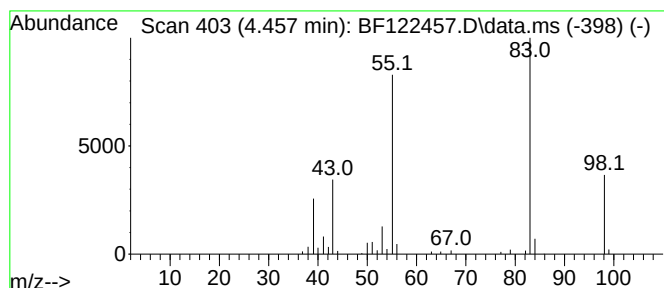
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.457	3.10 ng	150770	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3			3-Hexen-2-one	98	C6H10O	000763-93-9	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80



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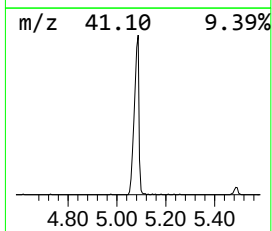
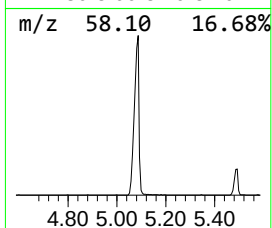
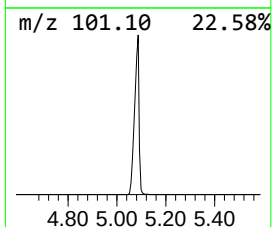
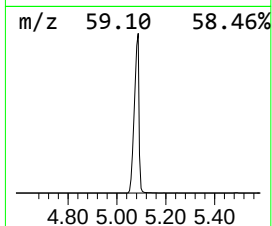
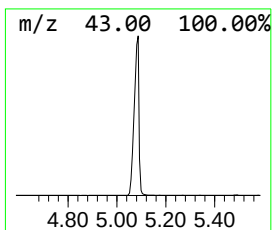
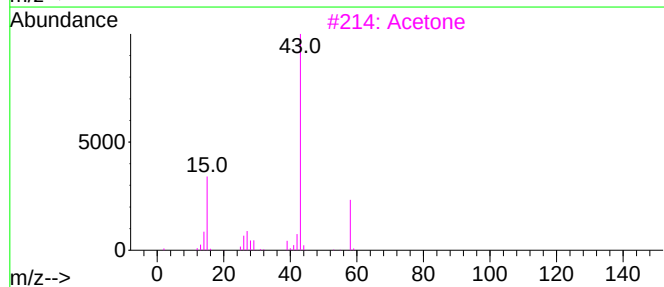
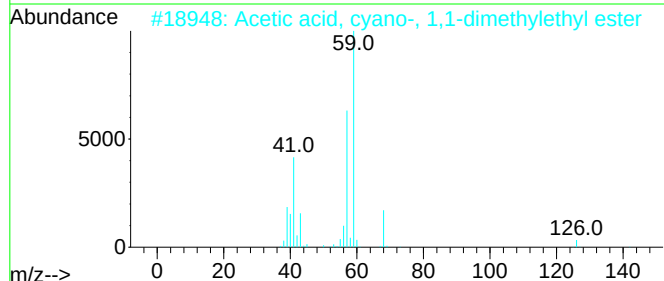
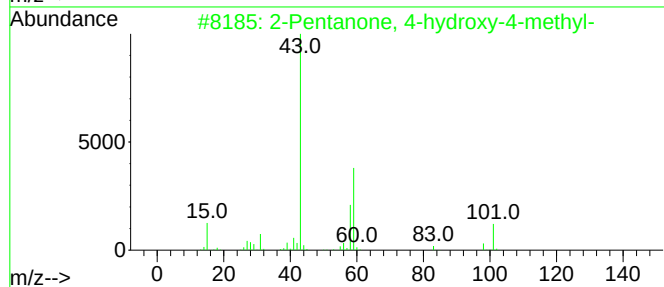
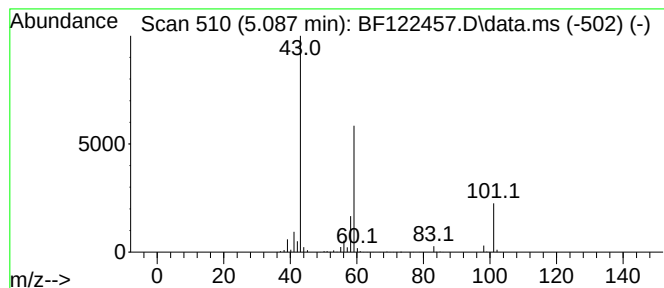
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.087	56.65 ng	2754540	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Acetone	58	C3H6O	000067-64-1	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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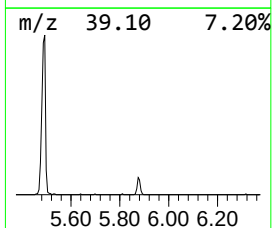
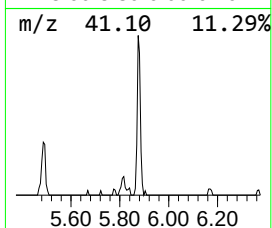
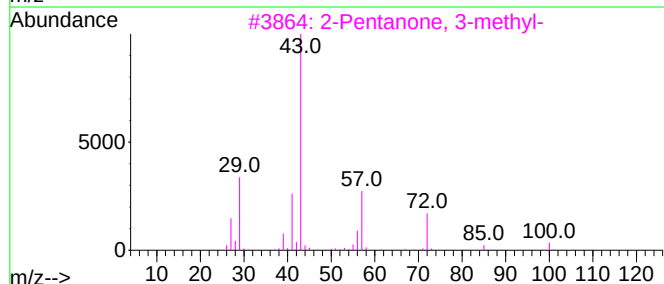
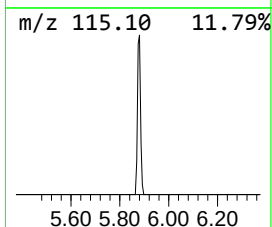
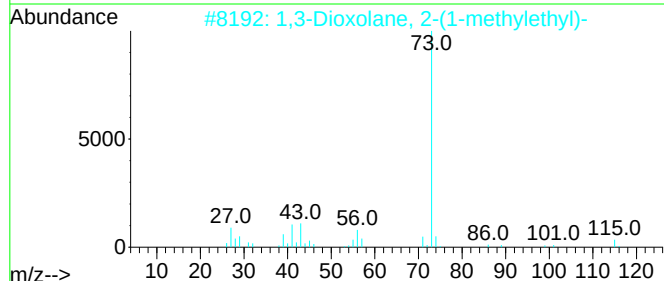
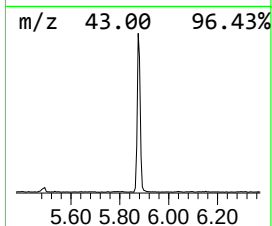
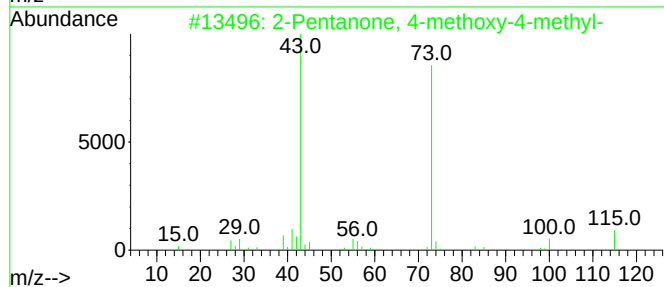
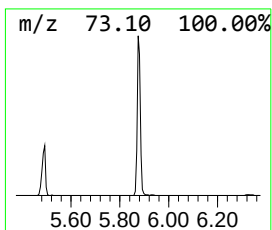
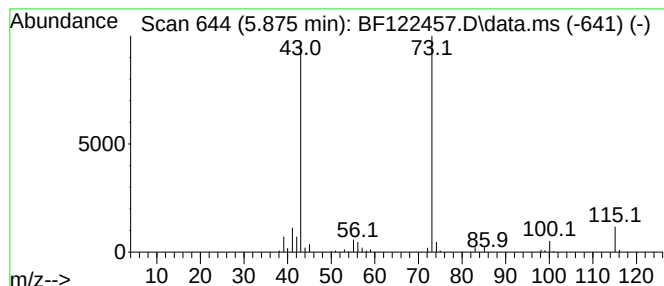
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	5.01 ng	243361	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83		
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	32		
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10		
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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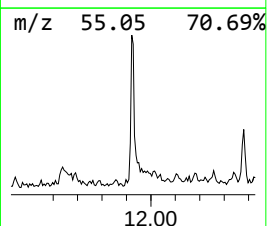
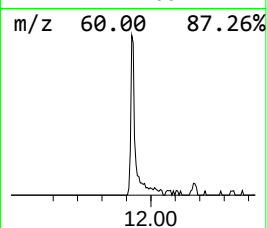
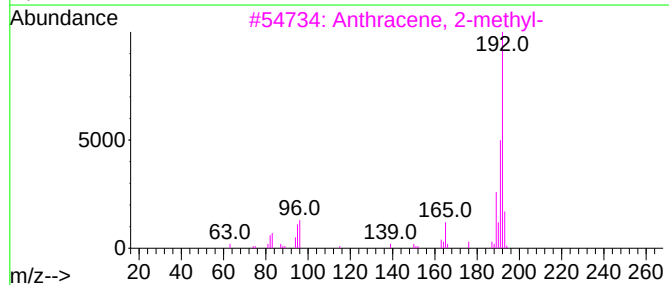
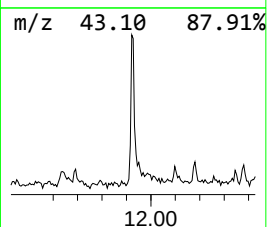
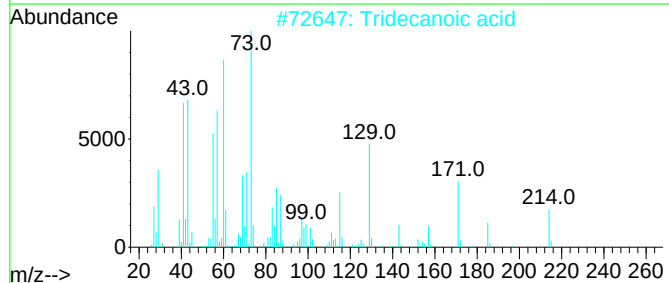
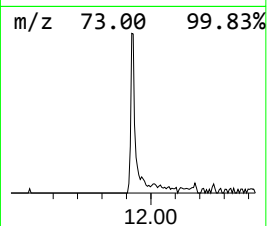
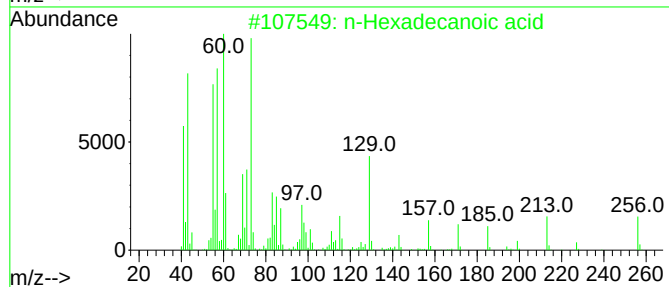
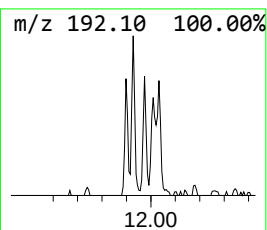
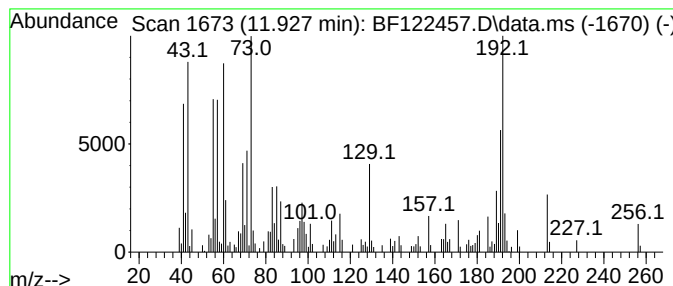
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	3.13 ng	193281	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Anthracene, 2-methyl-	192	C15H12	000613-12-7	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122457.D
Acq On : 23 Nov 2020 20:26
Operator : JU/CG
Sample : L4876-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
TB-2D

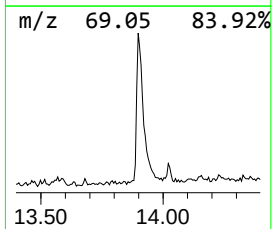
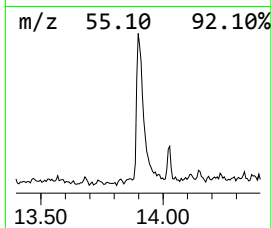
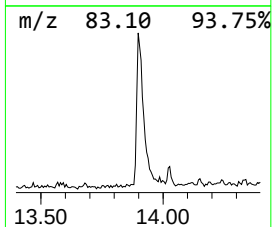
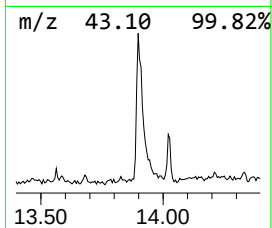
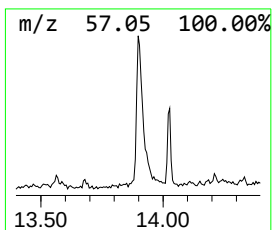
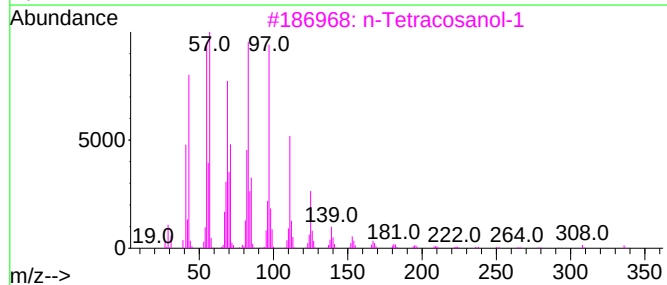
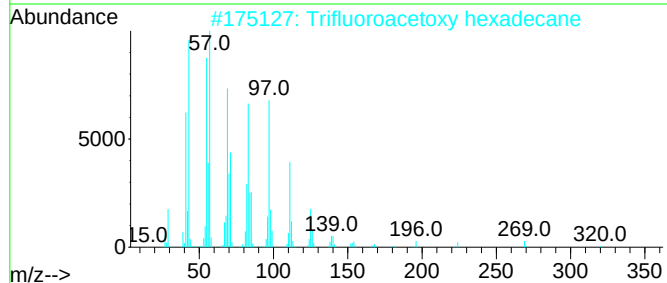
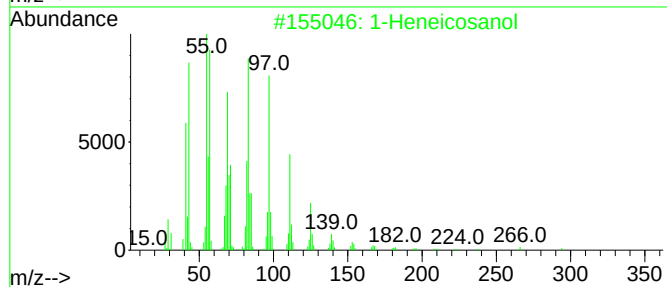
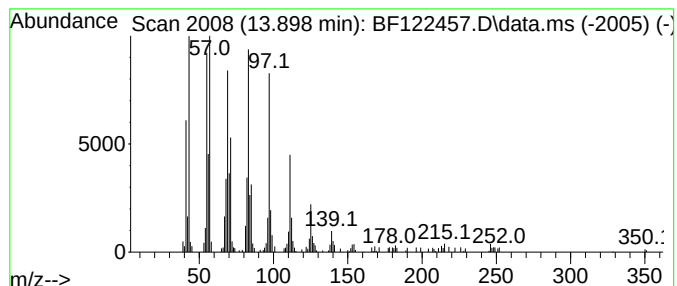
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	4.88 ng	445772	Chrysene-d12	14.039

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122457.D
Acq On : 23 Nov 2020 20:26
Operator : JU/CG
Sample : L4876-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TB-2D

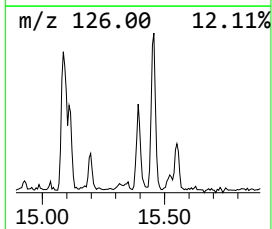
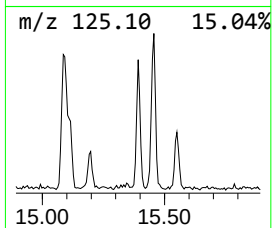
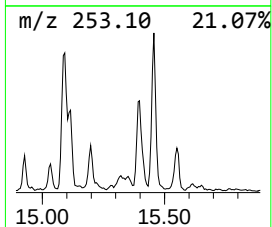
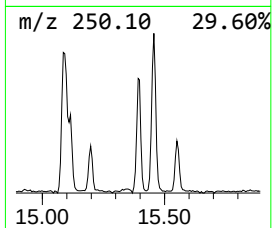
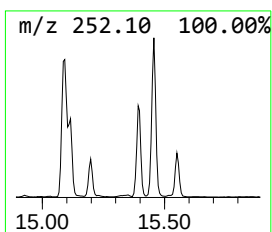
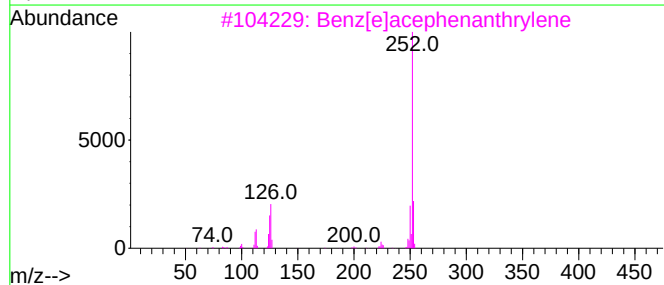
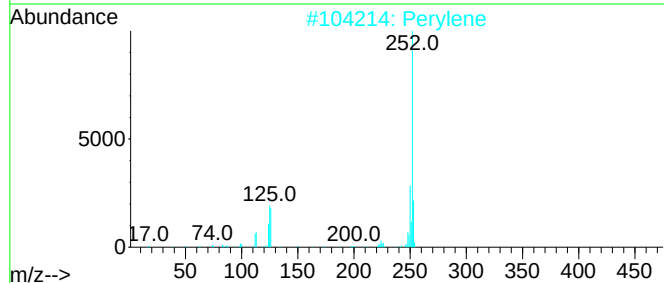
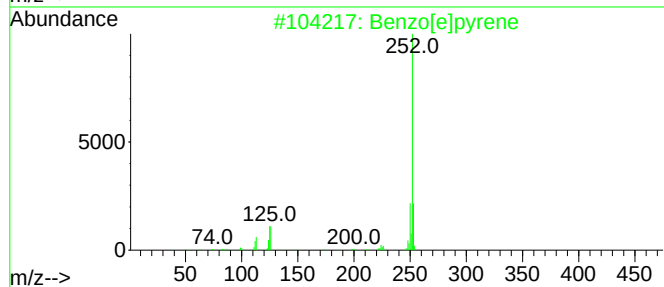
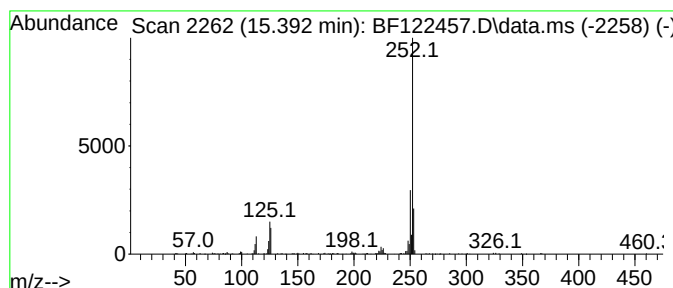
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	4.51 ng	326534	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Perylene	252	C20H12	000198-55-0	96
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	93
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122457.D
Acq On : 23 Nov 2020 20:26
Operator : JU/CG
Sample : L4876-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TB-2D

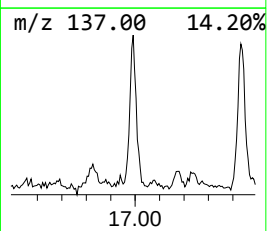
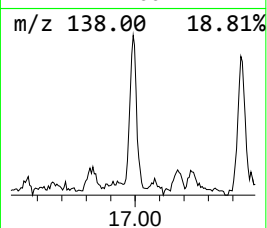
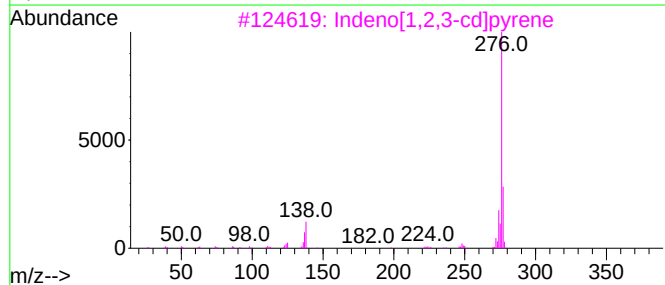
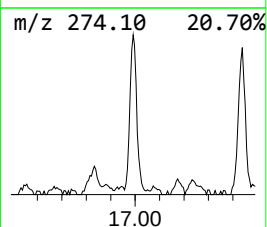
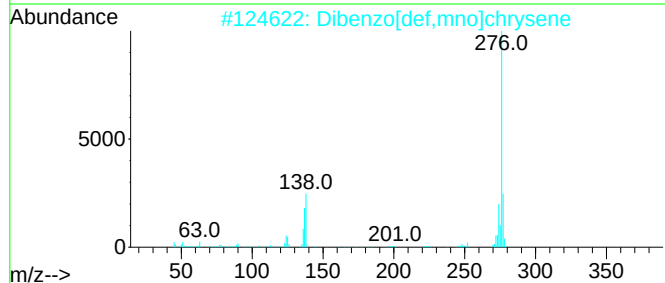
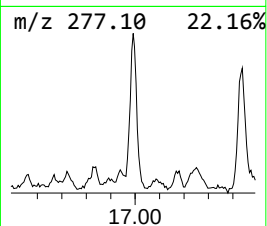
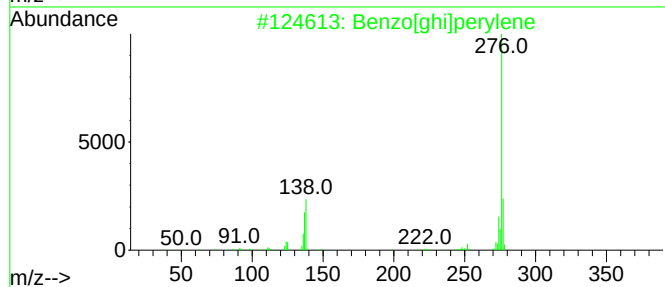
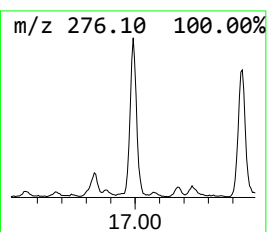
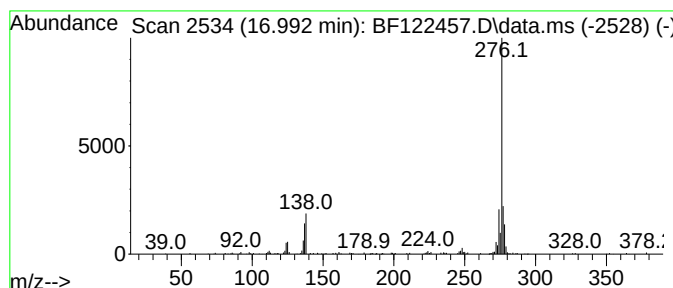
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.992	4.96 ng	359009	Perylene-d12	15.521

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[ghi]perylene	276	C22H12	000191-24-2	97
2			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	97
3			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	95
4			Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	52
5			Phosphoric acid, 4-methoxy-2-(me...	276	C11H17O6P	094420-71-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112320\
Data File : BF122457.D
Acq On : 23 Nov 2020 20:26
Operator : JU/CG
Sample : L4876-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TB-2D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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
Butane, 2-metho...	2.151	12.3	ng	598809	1	6.863	972420	20.0
3-Penten-2-one,...	4.457	3.1	ng	150770	1	6.863	972420	20.0
2-Pentanone, 4-...	5.087	56.6	ng	2754540	1	6.863	972420	20.0
2-Pentanone, 4-...	5.875	5.0	ng	243361	1	6.863	972420	20.0
n-Hexadecanoic ...	11.927	3.1	ng	193281	4	11.398	1234190	20.0
1-Heneicosanol	13.898	4.9	ng	445772	5	14.039	1828070	20.0
Benzo[e]pyrene	15.392	4.5	ng	326534	6	15.521	1447940	20.0
Dibenzo[def,mno...	16.992	5.0	ng	359009	6	15.521	1447940	20.0