

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092922\
 Data File : BF130474.D
 Acq On : 29 Sep 2022 19:16
 Operator : CG\JU
 Sample : N4868-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 ROLL-OFF-349-ETGI

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.157	348	352	359	rBV	55896	71029	2.58%	0.341%
2	4.834	461	467	486	rVB	1026086	1519415	55.25%	7.294%
3	5.251	534	538	549	rBV	2218872	2283133	83.02%	10.960%
4	5.651	602	606	613	rVB	105358	95820	3.48%	0.460%
5	6.287	709	714	717	rBV	2269344	2249783	81.81%	10.800%
6	6.640	770	774	777	rBV	643970	535662	19.48%	2.571%
7	7.204	865	870	873	rBV	1488372	1522457	55.36%	7.308%
8	7.839	974	978	988	rBV2	82402	242244	8.81%	1.163%
9	7.922	988	992	995	rVB	723994	660783	24.03%	3.172%
10	8.998	1169	1175	1178	rBV	3250541	2750134	100.00%	13.202%
11	9.669	1282	1289	1292	rBV	853409	678029	24.65%	3.255%
12	10.457	1419	1423	1426	rBV	1611061	1311351	47.68%	6.295%
13	10.580	1441	1444	1452	rBV2	27205	38840	1.41%	0.186%
14	11.151	1537	1541	1543	rBV	624735	570023	20.73%	2.736%
15	11.169	1543	1544	1549	rVV	184329	151957	5.53%	0.729%
16	11.222	1549	1553	1557	rVB	52368	49806	1.81%	0.239%
17	11.551	1605	1609	1613	rVB2	33041	33397	1.21%	0.160%
18	11.680	1628	1631	1636	rVB2	44182	49909	1.81%	0.240%
19	11.757	1641	1644	1647	rBV	47453	48991	1.78%	0.235%
20	12.357	1742	1746	1750	rBV	488101	399732	14.54%	1.919%
21	12.586	1779	1785	1788	rBV	342453	387999	14.11%	1.863%
22	12.733	1807	1810	1814	rVB	2057566	1839410	66.88%	8.830%
23	12.804	1817	1822	1826	rBV2	24727	39328	1.43%	0.189%
24	12.916	1838	1841	1844	rVB	56587	53926	1.96%	0.259%
25	12.980	1849	1852	1854	rVB	46596	39273	1.43%	0.189%
26	13.016	1854	1858	1860	rBV2	41018	41933	1.52%	0.201%
27	13.416	1924	1926	1931	rVB	28215	33107	1.20%	0.159%
28	13.527	1940	1945	1948	rBV2	56085	65608	2.39%	0.315%
29	13.627	1959	1962	1967	rVB	38822	43234	1.57%	0.208%
30	13.774	1979	1987	1990	rBV3	769431	995531	36.20%	4.779%
31	13.804	1990	1992	1995	rVB	225761	180521	6.56%	0.867%
32	13.880	2001	2005	2008	rBV2	56386	59911	2.18%	0.288%
33	14.168	2051	2054	2057	rVB	36983	35670	1.30%	0.171%
34	14.257	2066	2069	2072	rBV4	31431	38713	1.41%	0.186%
35	14.692	2140	2143	2147	rVB6	28903	34915	1.27%	0.168%
36	14.780	2154	2158	2161	rBV	273630	366171	13.31%	1.758%

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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-BF091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.051	2201	2204	2210	rVB	143221	166343	6.05%	0.798%
38	15.110	2210	2214	2219	rVB	206318	246158	8.95%	1.182%
39	15.168	2219	2224	2227	rBV	477348	540793	19.66%	2.596%
40	16.480	2442	2447	2455	rVB2	107587	198930	7.23%	0.955%
41	16.874	2509	2514	2525	rVB	86857	161974	5.89%	0.778%

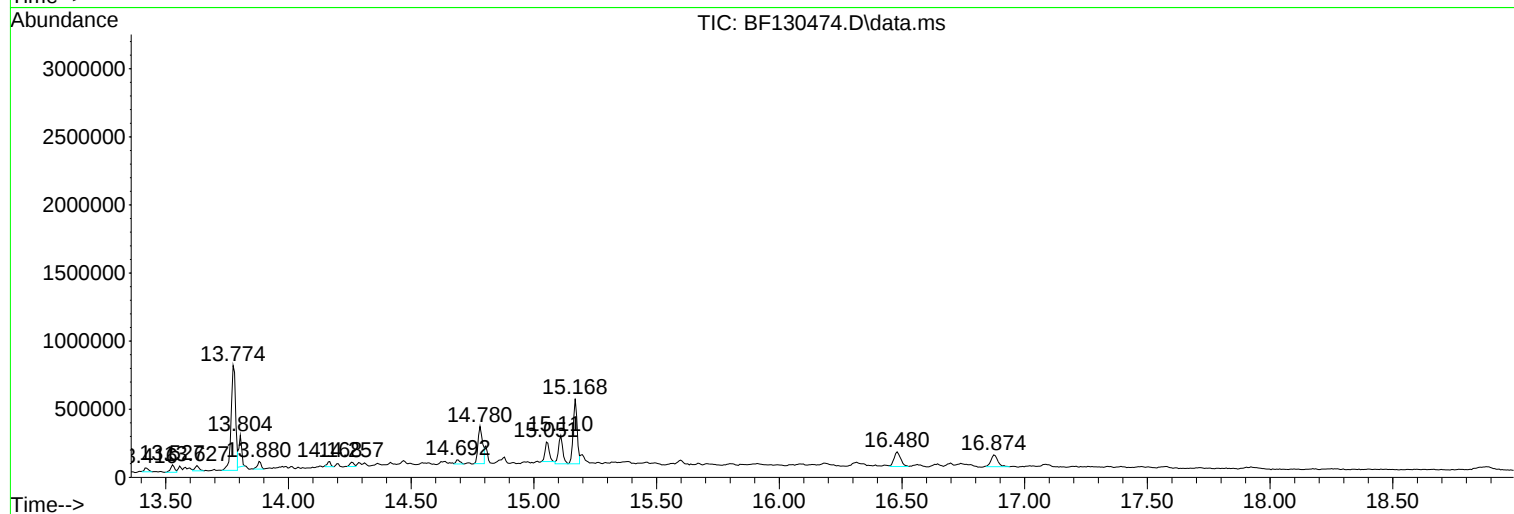
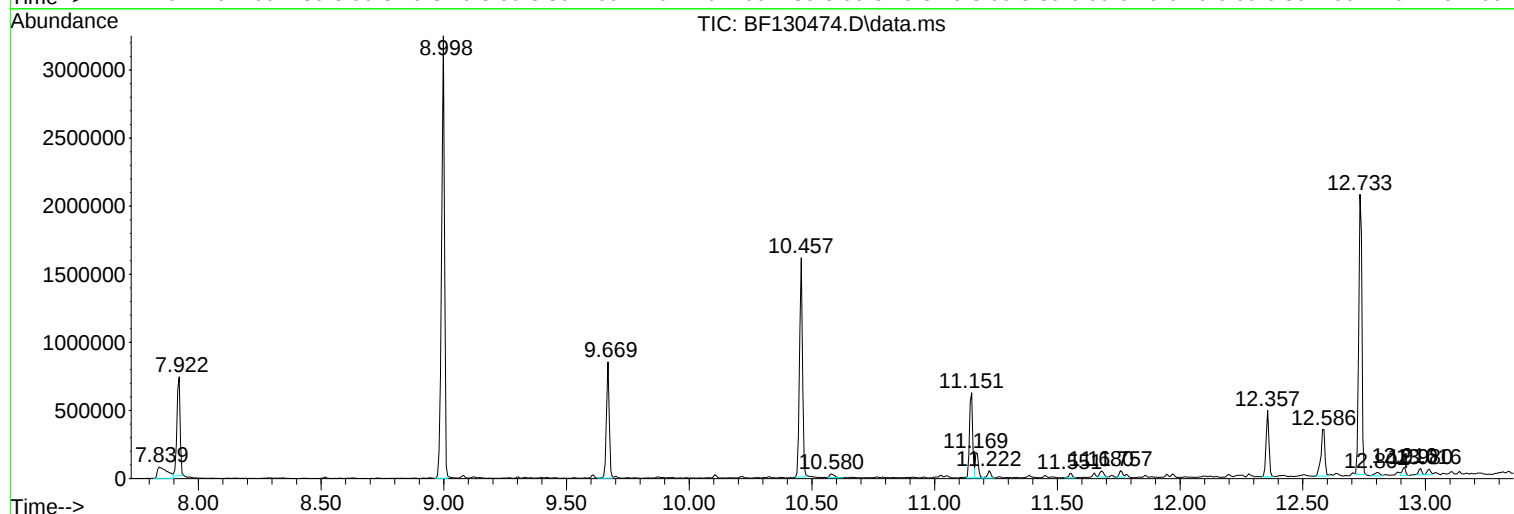
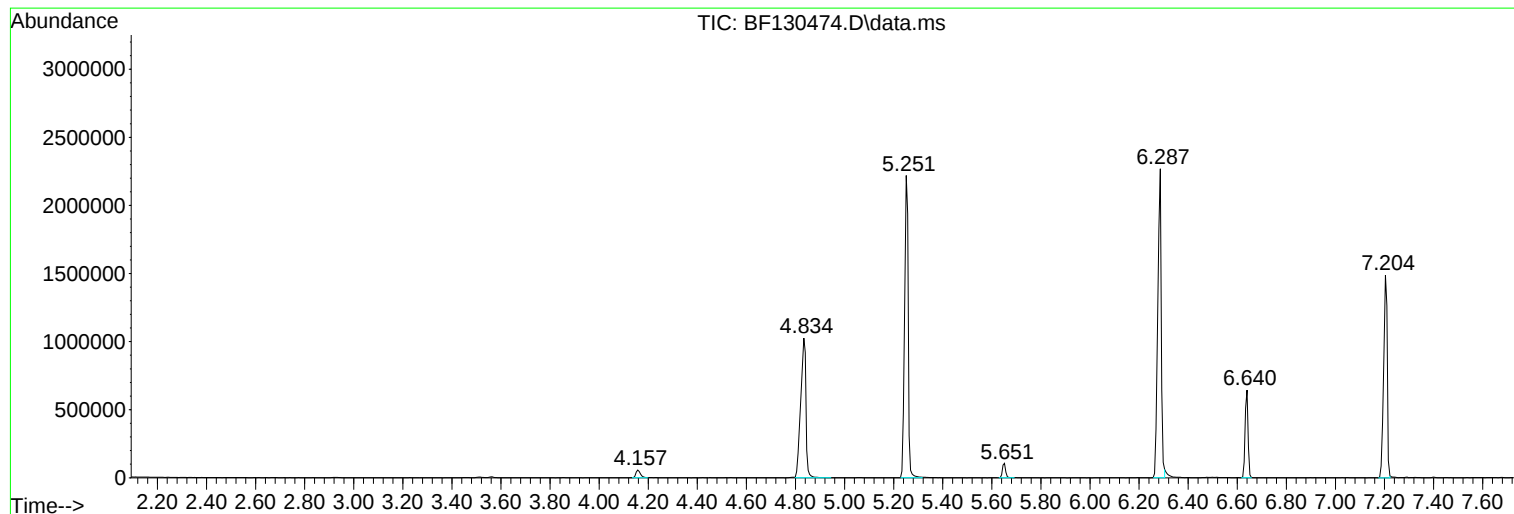
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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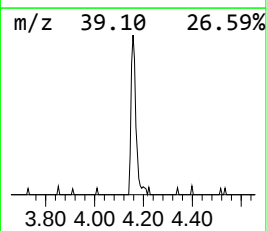
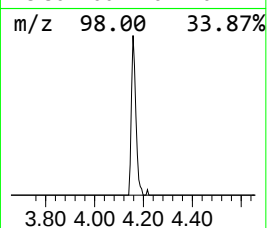
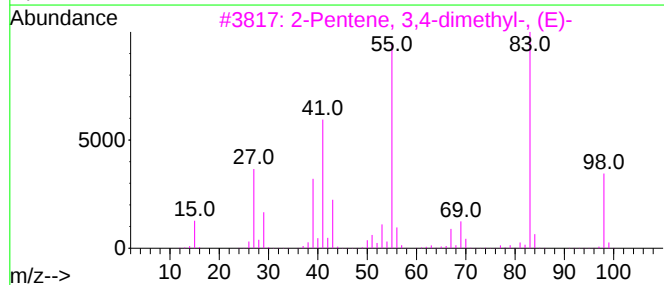
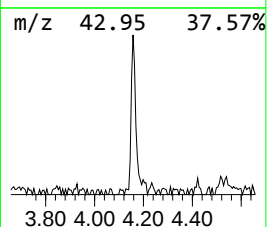
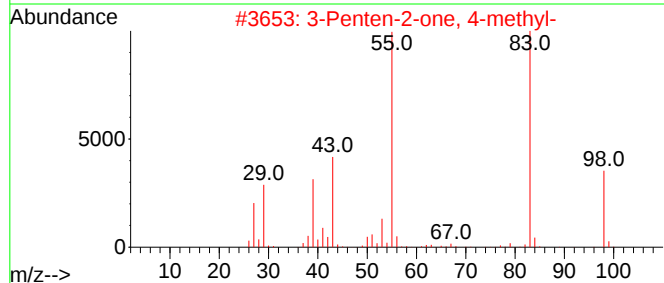
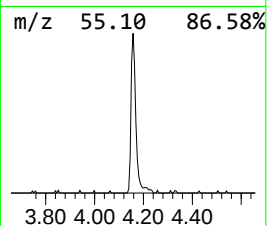
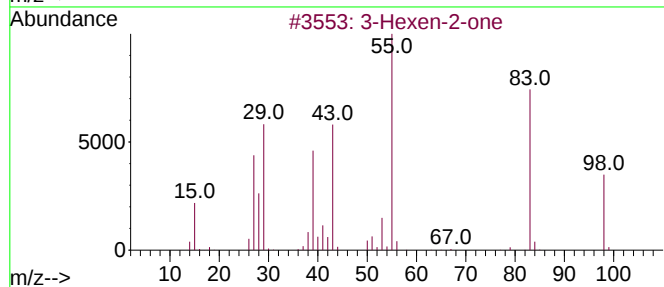
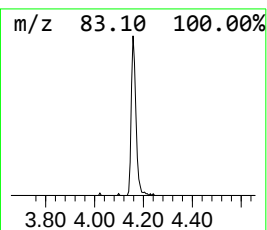
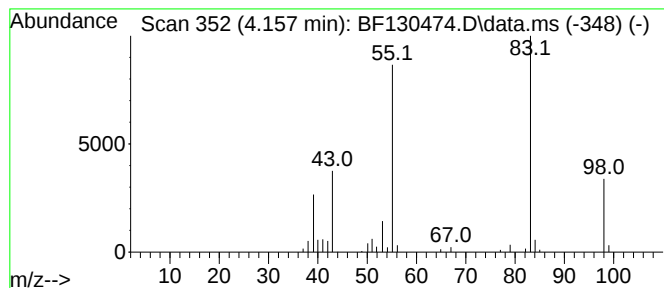
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.157	2.65 ng	71029	1,4-Dichlorobenzene-d4	6.640

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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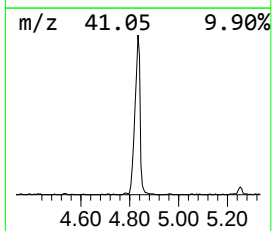
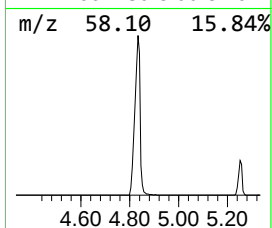
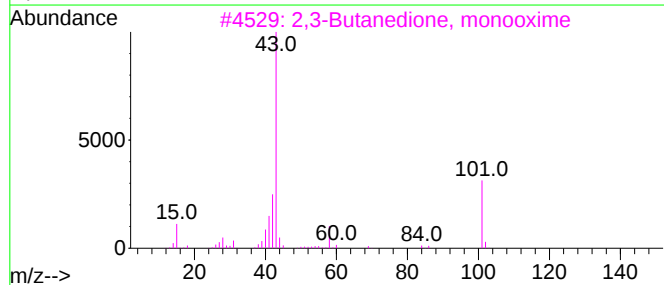
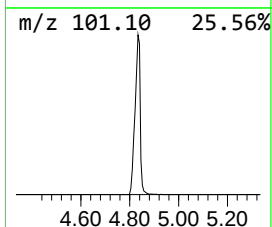
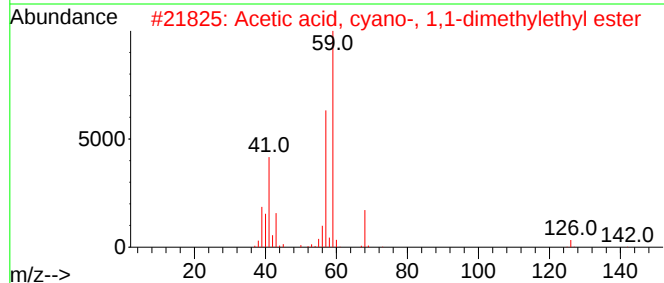
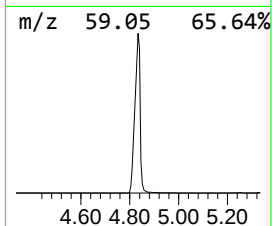
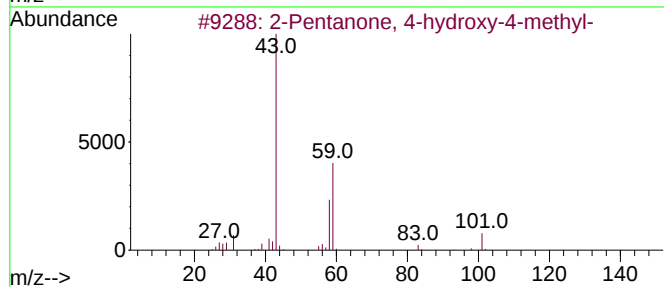
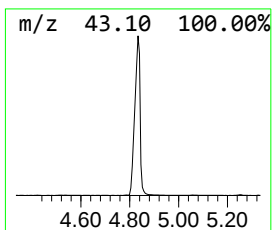
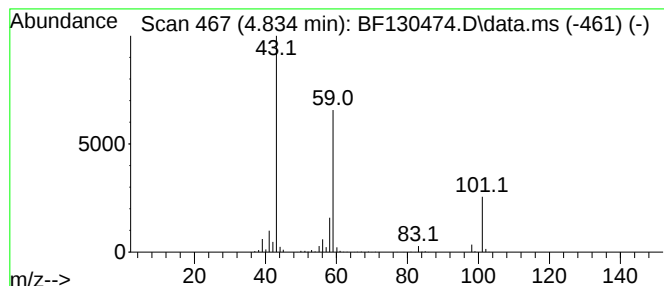
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.834	56.73 ng	1519420	1,4-Dichlorobenzene-d4			6.640
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	17
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
5	(+) -4-Amino-4,5-dihydro-2(3H)-f...		101	C4H7NO2	016504-58-8	9



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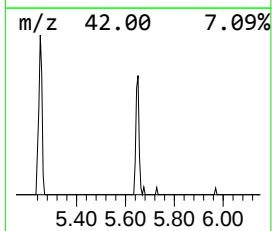
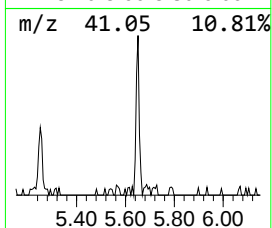
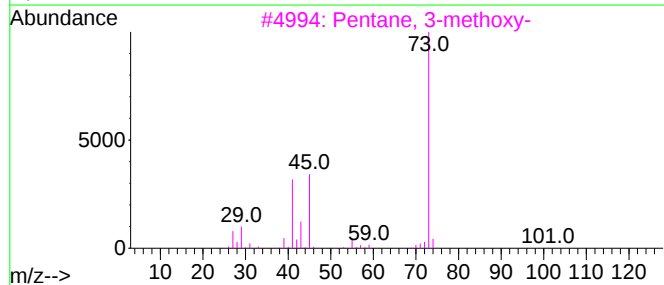
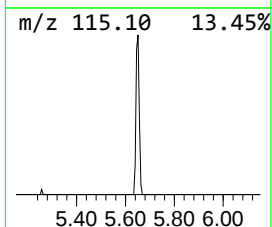
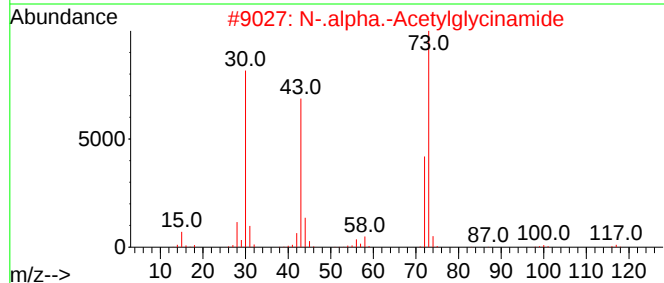
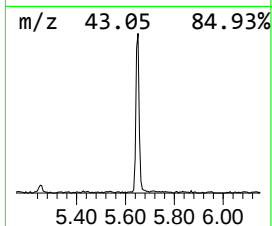
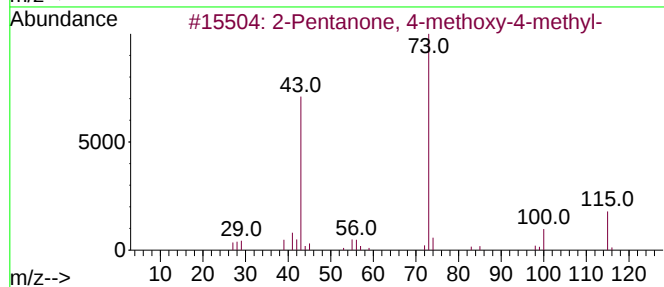
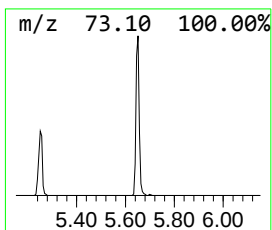
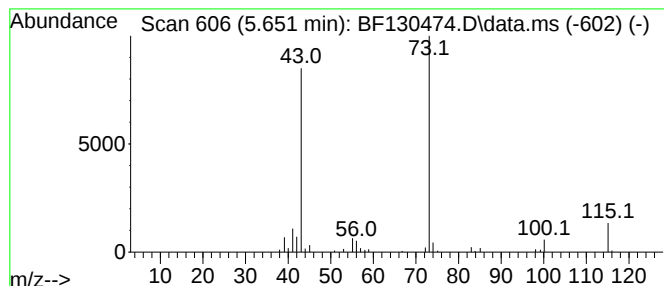
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.651	3.58 ng	95820	1,4-Dichlorobenzene-d4			6.640
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide		116	C4H8N2O2	002620-63-5	47
3	Pentane, 3-methoxy-		102	C6H14O	036839-67-5	12
4	4-Penten-2-one, 4-methyl-		98	C6H10O	003744-02-3	10
5	1,3-Dioxolane, 2-(1-methylethyl)-		116	C6H12O2	000822-83-3	10



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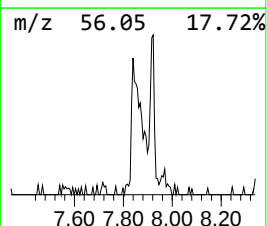
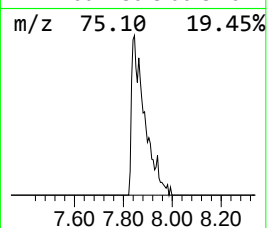
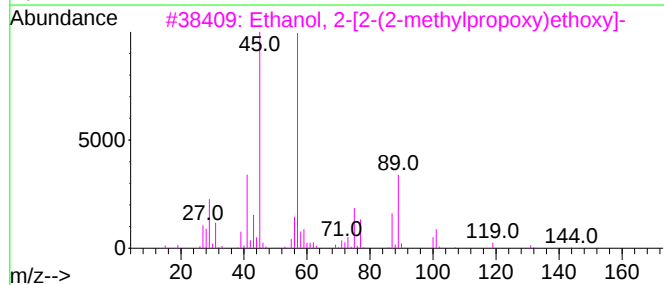
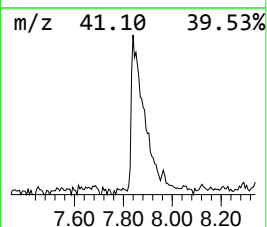
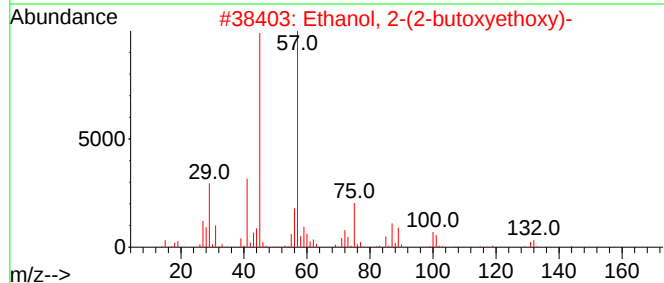
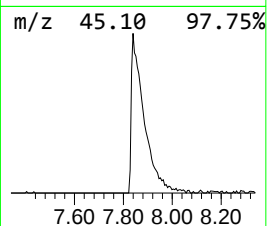
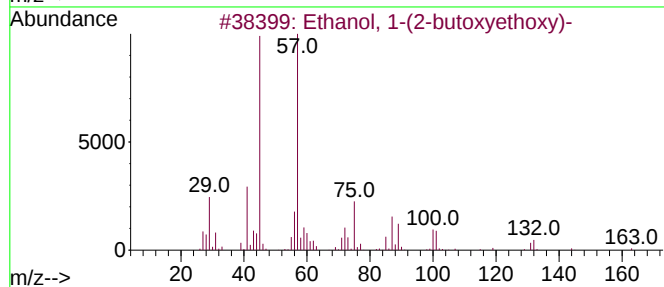
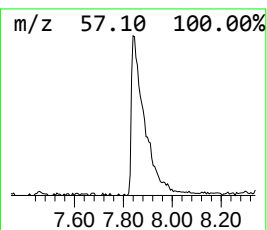
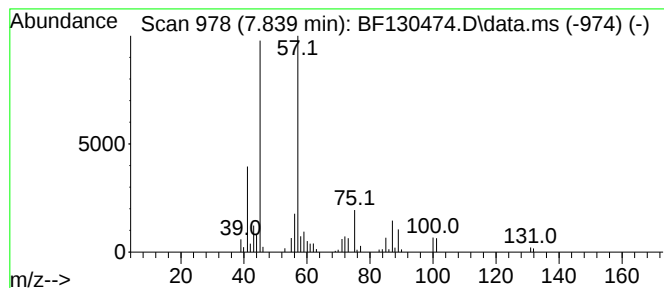
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.839	7.33 ng	242244	Naphthalene-d8	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	47



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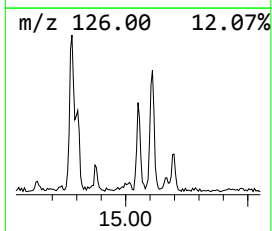
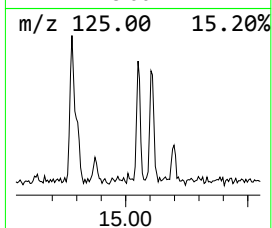
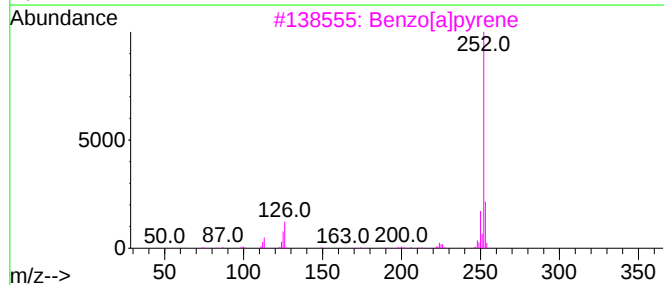
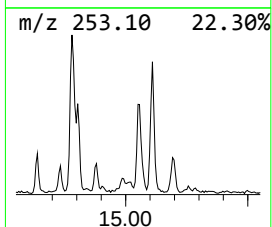
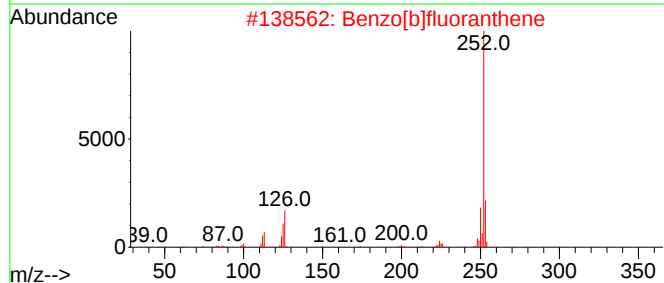
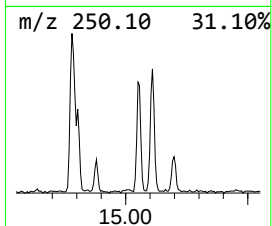
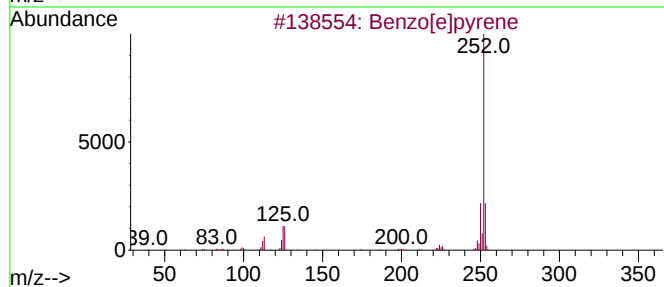
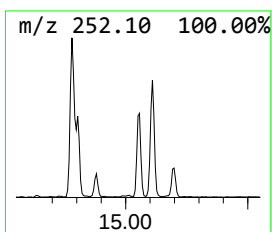
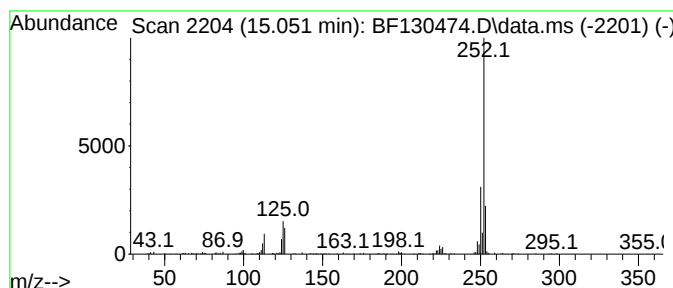
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.051	6.15 ng	166343	Perylene-d12	15.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	94
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
3			Benzo[a]pyrene	252	C20H12	000050-32-8	93
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092922\
Data File : BF130474.D
Acq On : 29 Sep 2022 19:16
Operator : CG\JU
Sample : N4868-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ROLL-OFF-349-ETGI

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.157	2.6	ng	71029	1	6.640	535662	20.0
2-Pentanone, 4-...	4.834	56.7	ng	1519420	1	6.640	535662	20.0
2-Pentanone, 4-...	5.651	3.6	ng	95820	1	6.640	535662	20.0
Ethanol, 1-(2-b...	7.839	7.3	ng	242244	2	7.922	660783	20.0
Benzo[e]pyrene	15.051	6.2	ng	166343	6	15.168	540793	20.0