

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
 Data File : BF138376.D
 Acq On : 27 Jun 2024 20:09
 Operator : CG\JU
 Sample : P3076-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 7-E-1

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138376.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	8	17	22	rBV	2319930	3074195	76.55%	8.468%
2	2.293	29	35	41	rBV2	38578	52709	1.31%	0.145%
3	3.428	222	228	253	rBV	186971	434139	10.81%	1.196%
4	5.104	509	513	521	rVB	255149	306557	7.63%	0.844%
5	5.510	578	582	585	rBV	4205166	3652922	90.95%	10.062%
6	6.516	748	753	756	rBV	3912543	3558197	88.60%	9.801%
7	6.881	811	815	818	rBV	1594378	1258009	31.32%	3.465%
8	7.440	905	910	913	rBV	2564577	2355730	58.66%	6.489%
9	7.693	950	953	956	rVB	108522	81334	2.03%	0.224%
10	8.157	1029	1032	1035	rBV	1832716	1547689	38.54%	4.263%
11	8.469	1081	1085	1094	rBV	158410	144903	3.61%	0.399%
12	9.234	1211	1215	1218	rBV	5059491	4016192	100.00%	11.062%
13	9.910	1327	1330	1334	rBV	1711791	1413710	35.20%	3.894%
14	10.010	1342	1347	1351	rBV	1634685	1992322	49.61%	5.488%
15	10.698	1460	1464	1477	rBV	2184506	1862603	46.38%	5.130%
16	10.810	1479	1483	1490	rVB2	38524	52697	1.31%	0.145%
17	11.398	1579	1583	1585	rBV	1382726	1176254	29.29%	3.240%
18	11.422	1585	1587	1590	rVV	423964	329735	8.21%	0.908%
19	11.469	1590	1595	1598	rVB	72831	76228	1.90%	0.210%
20	11.922	1669	1672	1679	rBV2	252386	231784	5.77%	0.638%
21	12.010	1684	1687	1689	rBV	73204	65962	1.64%	0.182%
22	12.492	1764	1769	1773	rVB4	46915	59416	1.48%	0.164%
23	12.610	1785	1789	1792	rBV	753127	632972	15.76%	1.743%
24	12.704	1802	1805	1808	rBV	78726	80444	2.00%	0.222%
25	12.833	1822	1827	1833	rVB	584318	631202	15.72%	1.739%
26	12.980	1848	1852	1855	rBV	3955963	3300034	82.17%	9.090%
27	13.057	1860	1865	1868	rBV2	37531	71376	1.78%	0.197%
28	13.163	1881	1883	1885	rVB	72610	55392	1.38%	0.153%
29	13.874	2001	2004	2010	rBV2	261150	283820	7.07%	0.782%
30	14.033	2026	2031	2034	rBV2	1519717	1573222	39.17%	4.333%
31	14.057	2034	2035	2041	rVB	306651	225435	5.61%	0.621%
32	14.139	2046	2049	2052	rVB	59383	54106	1.35%	0.149%
33	14.504	2108	2111	2115	rBV4	53168	81784	2.04%	0.225%
34	15.074	2204	2208	2211	rBV	185125	288563	7.18%	0.795%
35	15.374	2256	2259	2265	rBV	97499	134165	3.34%	0.370%
36	15.439	2266	2270	2276	rVB	161781	211992	5.28%	0.584%

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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-BF061224.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.504	2276	2281	2285	rBV	785353	937433	23.34%	2.582%
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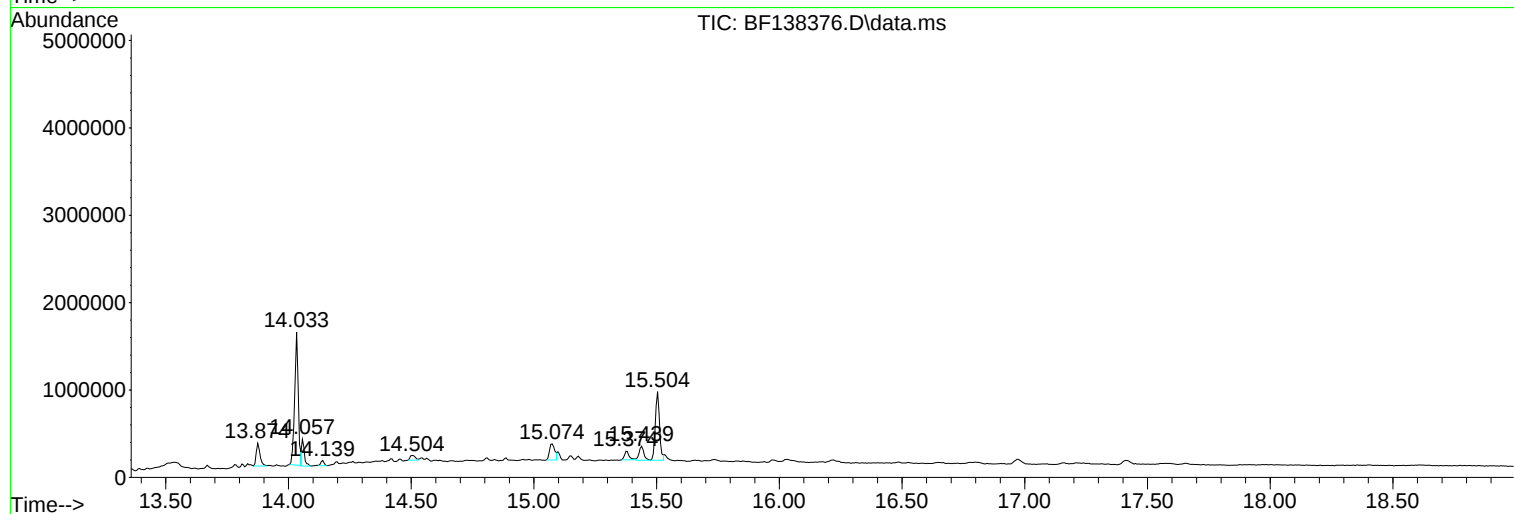
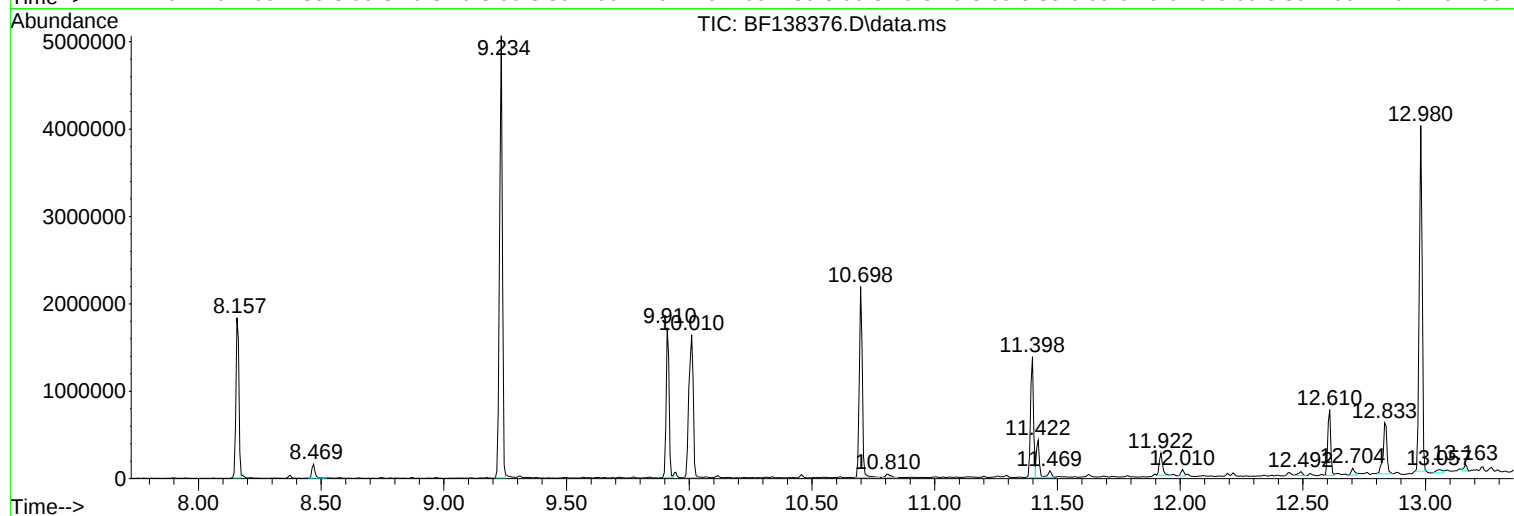
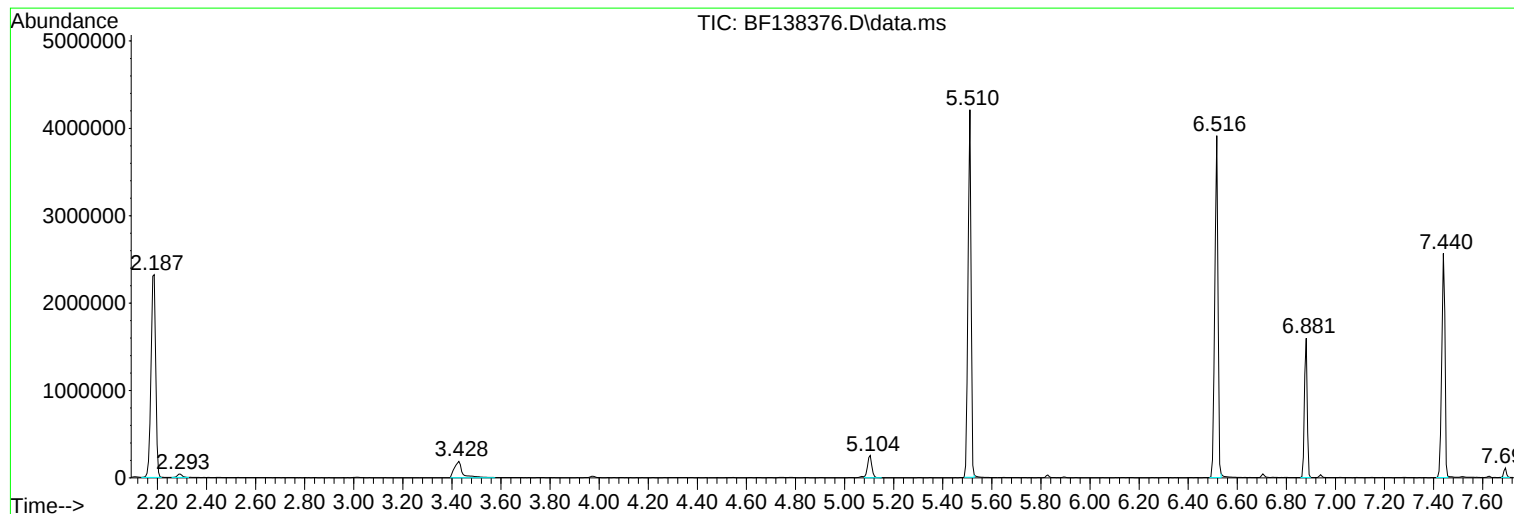
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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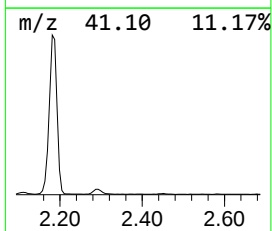
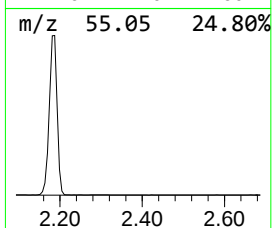
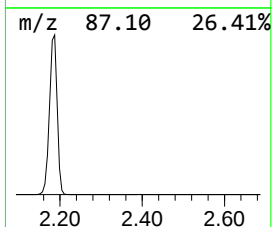
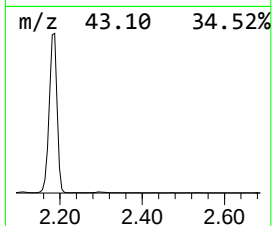
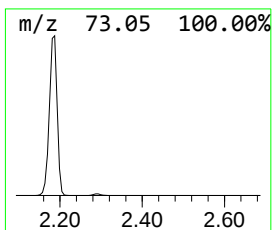
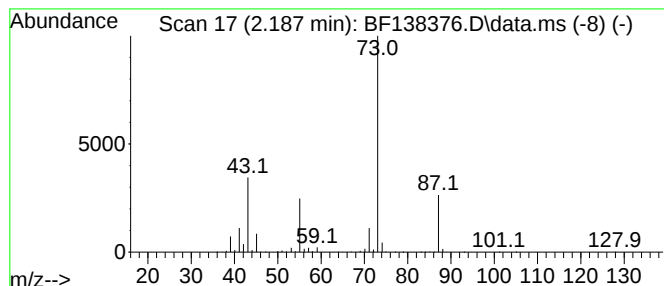
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.187	48.87 ng	3074200	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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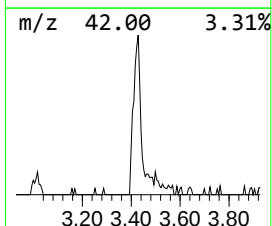
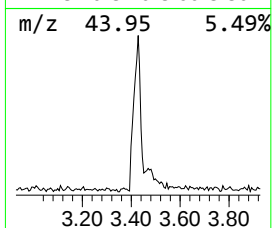
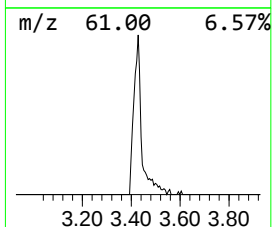
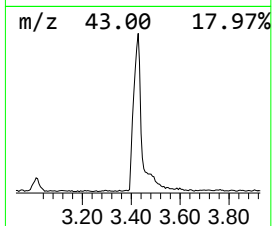
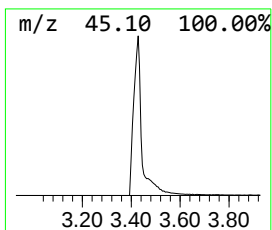
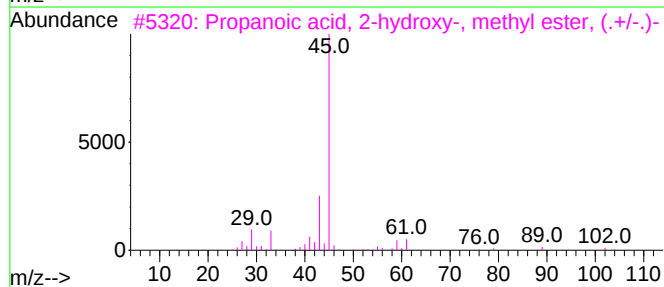
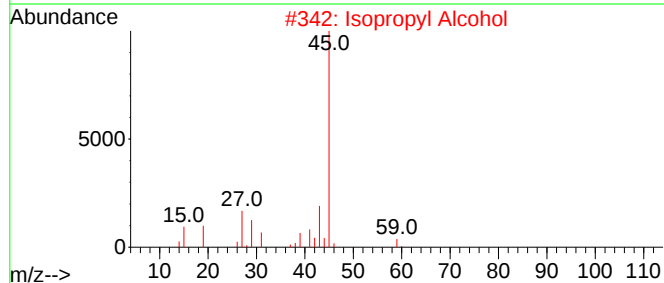
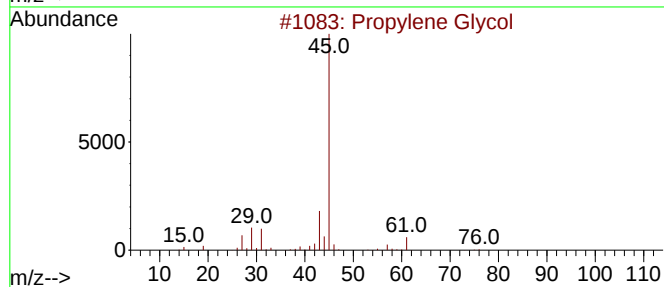
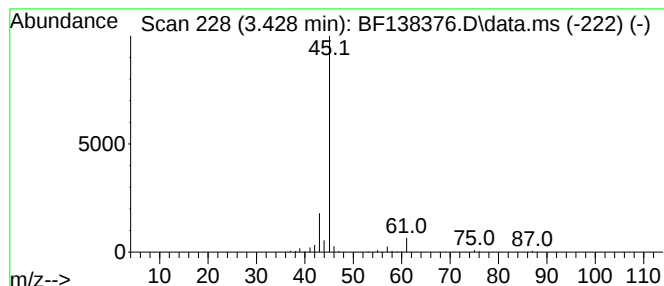
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.428	6.90 ng	434139	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	86
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	50
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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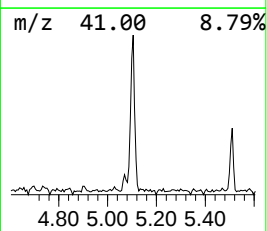
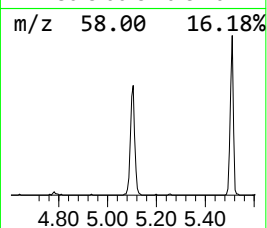
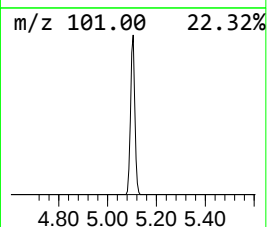
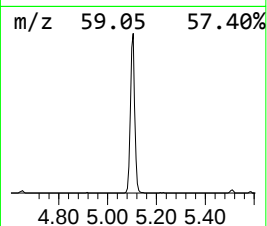
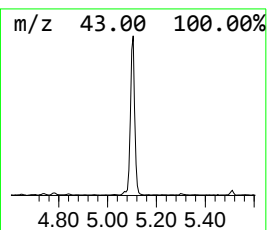
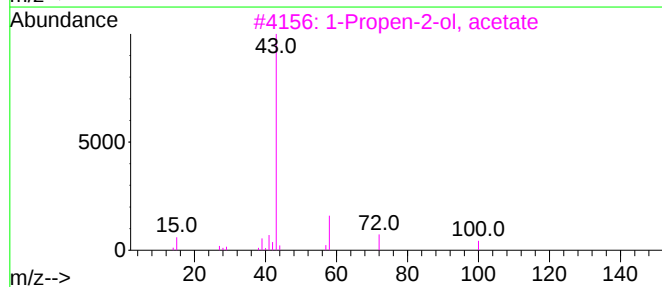
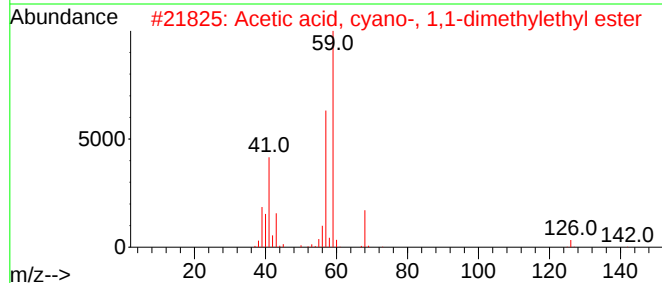
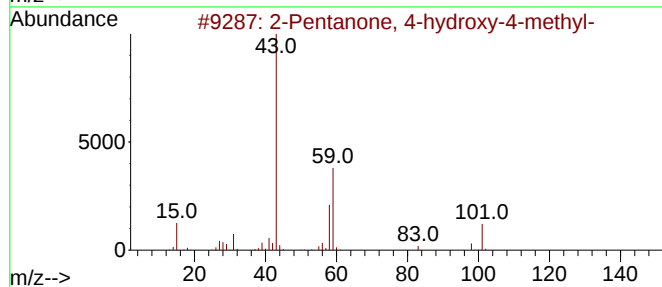
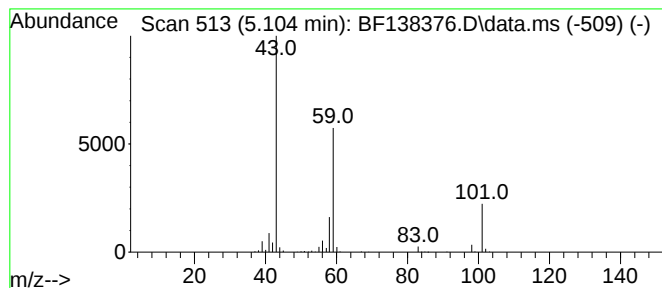
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.87 ng	306557	1,4-Dichlorobenzene-d4	6.881

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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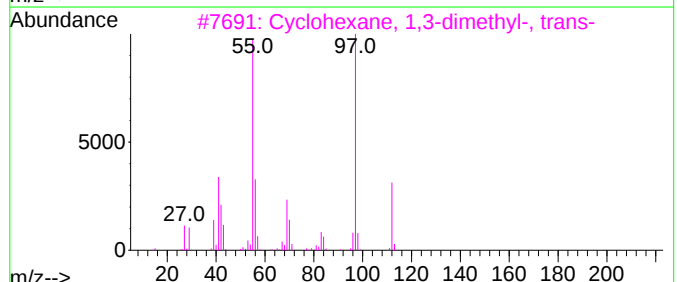
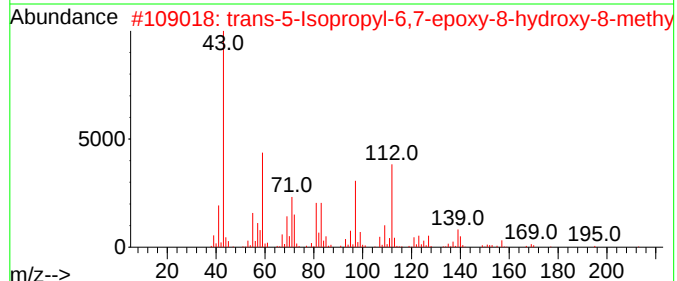
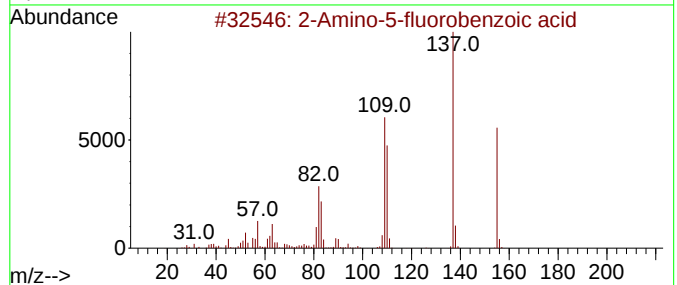
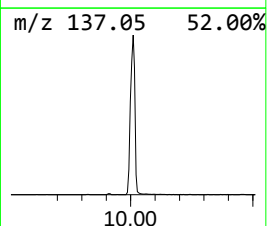
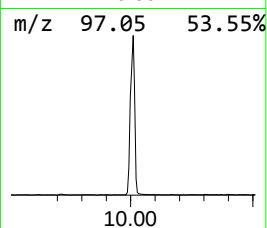
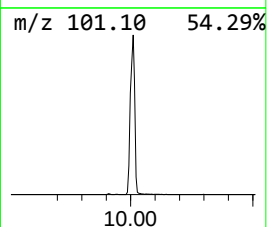
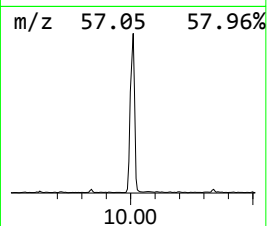
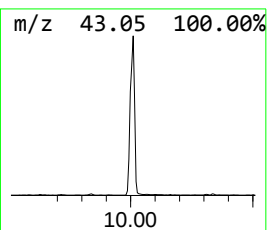
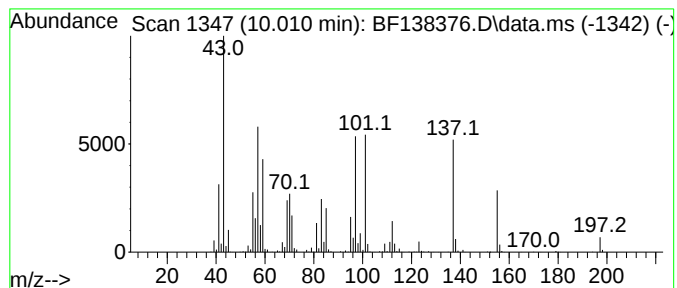
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown10.010 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	28.19 ng	1992320	Acenaphthene-d10	9.910

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Amino-5-fluorobenzoic acid	155	C7H6FN02	000446-08-2	14
2		trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
3		Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	11
4		Cyclohexane, 1,3-dimethyl-	112	C8H16	000591-21-9	11
5		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10



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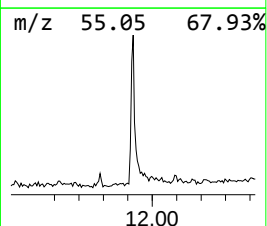
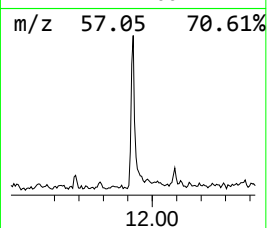
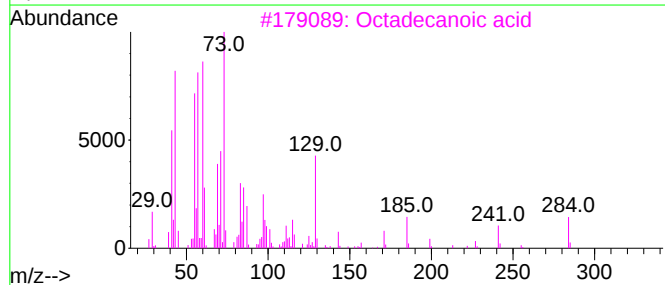
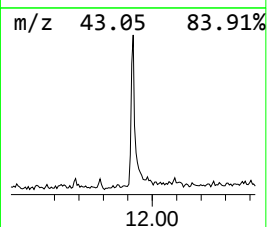
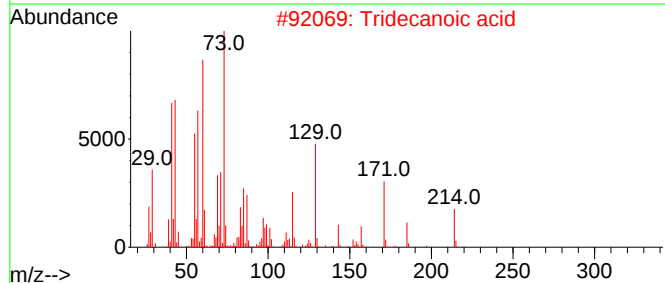
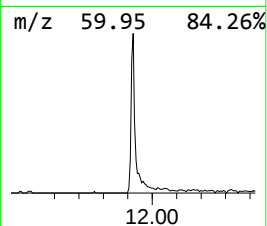
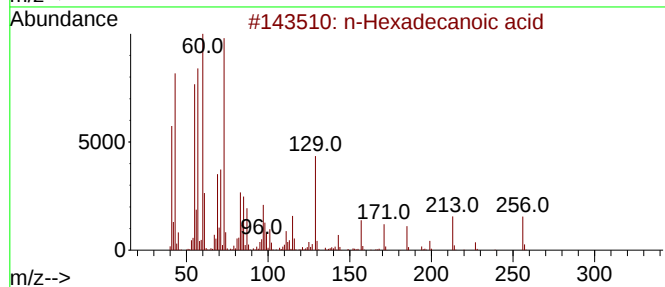
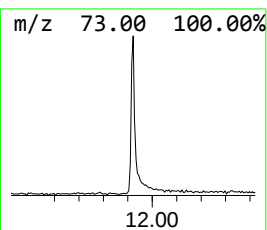
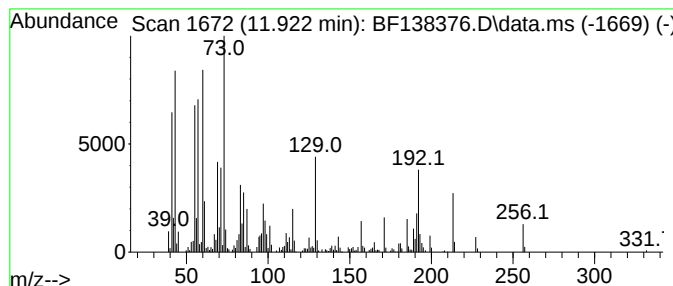
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.94 ng	231784	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138376.D
Acq On : 27 Jun 2024 20:09
Operator : CG\JU
Sample : P3076-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-E-1

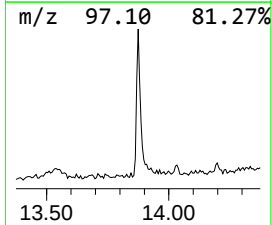
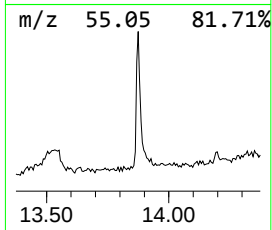
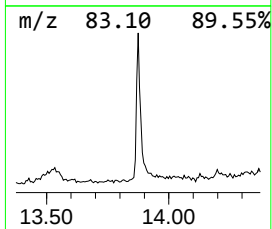
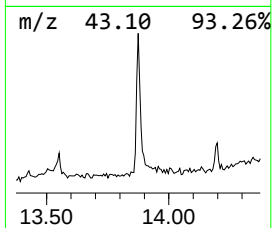
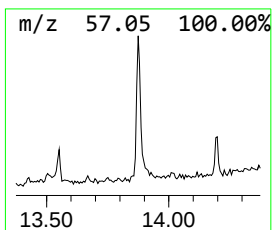
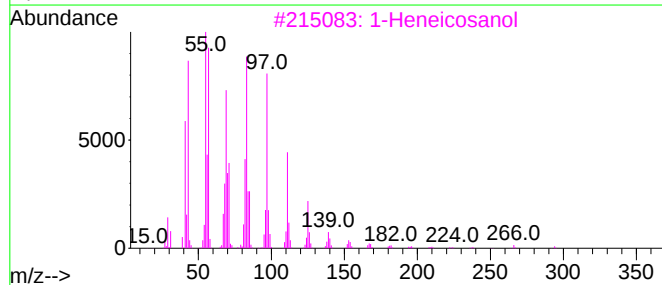
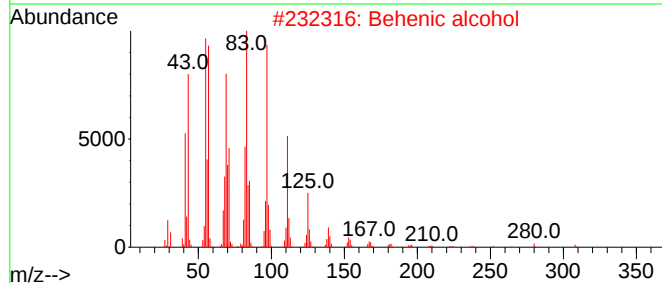
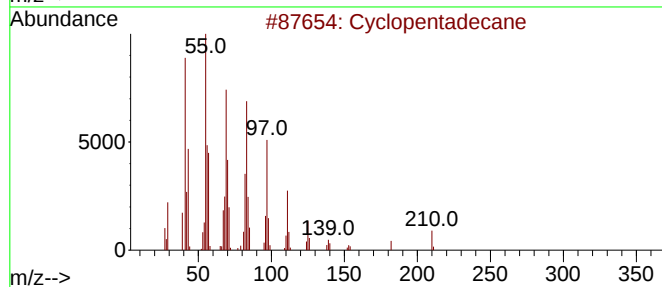
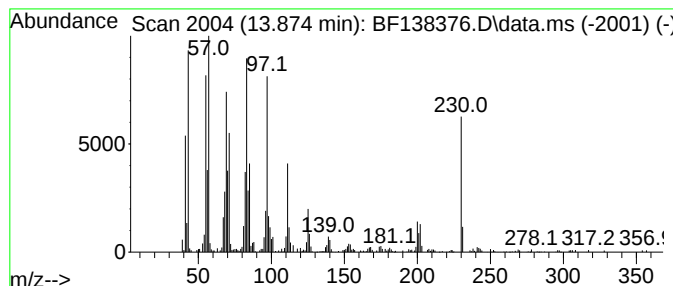
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	3.61 ng	283820	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	94
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			1-Heptacosanol	396	C27H56O	002004-39-9	93
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138376.D
Acq On : 27 Jun 2024 20:09
Operator : CG\JU
Sample : P3076-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-E-1

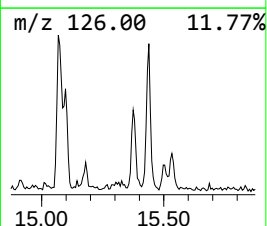
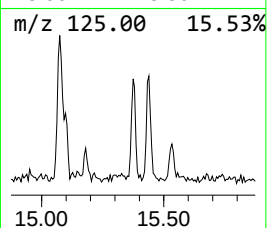
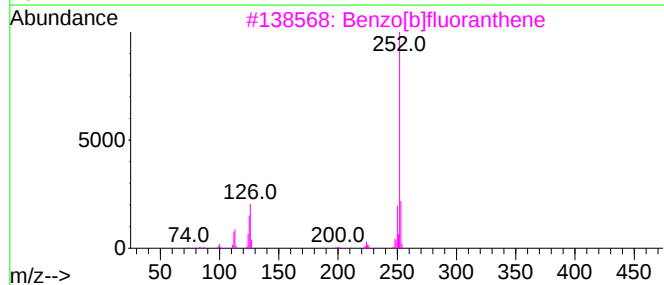
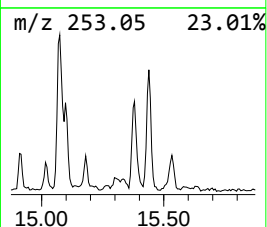
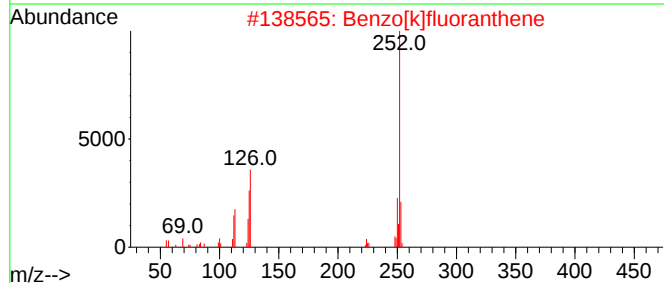
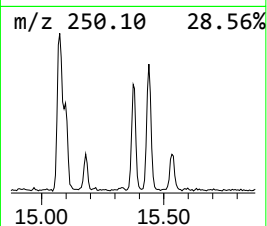
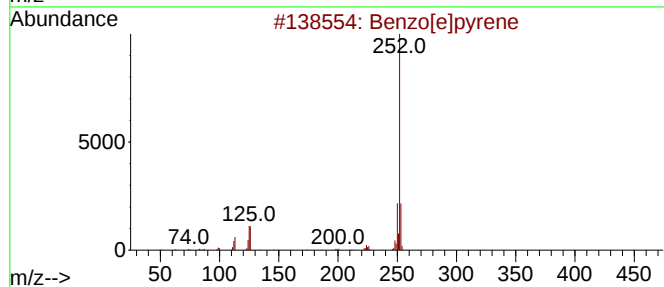
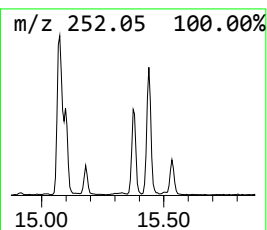
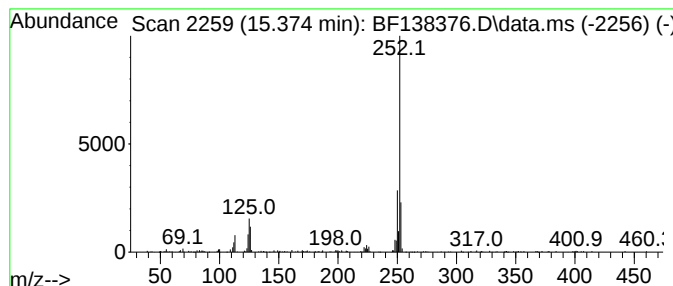
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.374	2.86 ng	134165	Perylene-d12	15.504

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	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	95
4			Benzo[a]pyrene	252	C20H12	000050-32-8	91
5			Perylene	252	C20H12	000198-55-0	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062724\
Data File : BF138376.D
Acq On : 27 Jun 2024 20:09
Operator : CG\JU
Sample : P3076-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
7-E-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.187	48.9	ng	3074200	1	6.881	1258010	20.0
Propylene Glycol	3.428	6.9	ng	434139	1	6.881	1258010	20.0
2-Pentanone, 4-...	5.104	4.9	ng	306557	1	6.881	1258010	20.0
unknown10.010	10.010	28.2	ng	1992320	3	9.910	1413710	20.0
n-Hexadecanoic ...	11.922	3.9	ng	231784	4	11.398	1176250	20.0
Cyclopentadecane	13.874	3.6	ng	283820	5	14.033	1573220	20.0
Benzo[e]pyrene	15.374	2.9	ng	134165	6	15.504	937433	20.0