

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092922\
 Data File : BF130469.D
 Acq On : 29 Sep 2022 16:23
 Operator : CG\JU
 Sample : N4862-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A2720

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: BF130469.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.146	346	350	359	rBV	30917	40651	1.10%	0.213%
2	4.816	459	464	481	rVB	409701	497898	13.50%	2.607%
3	5.240	532	536	547	rBV	1490310	1372574	37.22%	7.188%
4	5.646	601	605	608	rBV	85268	77637	2.11%	0.407%
5	6.275	708	712	724	rBV	973578	909852	24.67%	4.765%
6	6.634	770	773	777	rBV	675793	614344	16.66%	3.217%
7	7.204	865	870	873	rBV	1674359	1869401	50.69%	9.789%
8	7.887	979	986	987	rBV4	27122	52150	1.41%	0.273%
9	7.922	987	992	995	rVB	852352	802766	21.77%	4.204%
10	8.998	1169	1175	1178	rBV	3982364	3688122	100.00%	19.313%
11	9.669	1284	1289	1292	rBV	1065836	899588	24.39%	4.711%
12	9.698	1292	1294	1297	rVB	71471	60985	1.65%	0.319%
13	10.110	1360	1364	1366	rVB	79238	72150	1.96%	0.378%
14	10.463	1418	1424	1427	rBV	2366035	2318426	62.86%	12.141%
15	10.581	1440	1444	1452	rVB2	147649	171161	4.64%	0.896%
16	10.939	1503	1505	1512	rVB	45976	48614	1.32%	0.255%
17	11.028	1517	1520	1522	rVV	101337	82204	2.23%	0.430%
18	11.057	1522	1525	1528	rVB3	42295	52456	1.42%	0.275%
19	11.151	1537	1541	1544	rVB	1000519	810250	21.97%	4.243%
20	11.451	1589	1592	1598	rVB	80599	70552	1.91%	0.369%
21	11.545	1604	1608	1613	rVB2	199186	189680	5.14%	0.993%
22	11.692	1630	1633	1636	rBV	152864	126103	3.42%	0.660%
23	11.857	1659	1661	1664	rVB	57903	43539	1.18%	0.228%
24	12.245	1725	1727	1731	rVB	45674	39727	1.08%	0.208%
25	12.475	1764	1766	1776	rVB8	38867	59304	1.61%	0.311%
26	12.739	1806	1811	1814	rBV	3360373	2913001	78.98%	15.254%
27	13.645	1962	1965	1971	rVB	44761	45973	1.25%	0.241%
28	13.780	1984	1988	1997	rBV	704435	658756	17.86%	3.450%
29	14.263	2067	2070	2074	rVB	40871	39817	1.08%	0.209%
30	15.168	2220	2224	2228	rBV	446844	468757	12.71%	2.455%

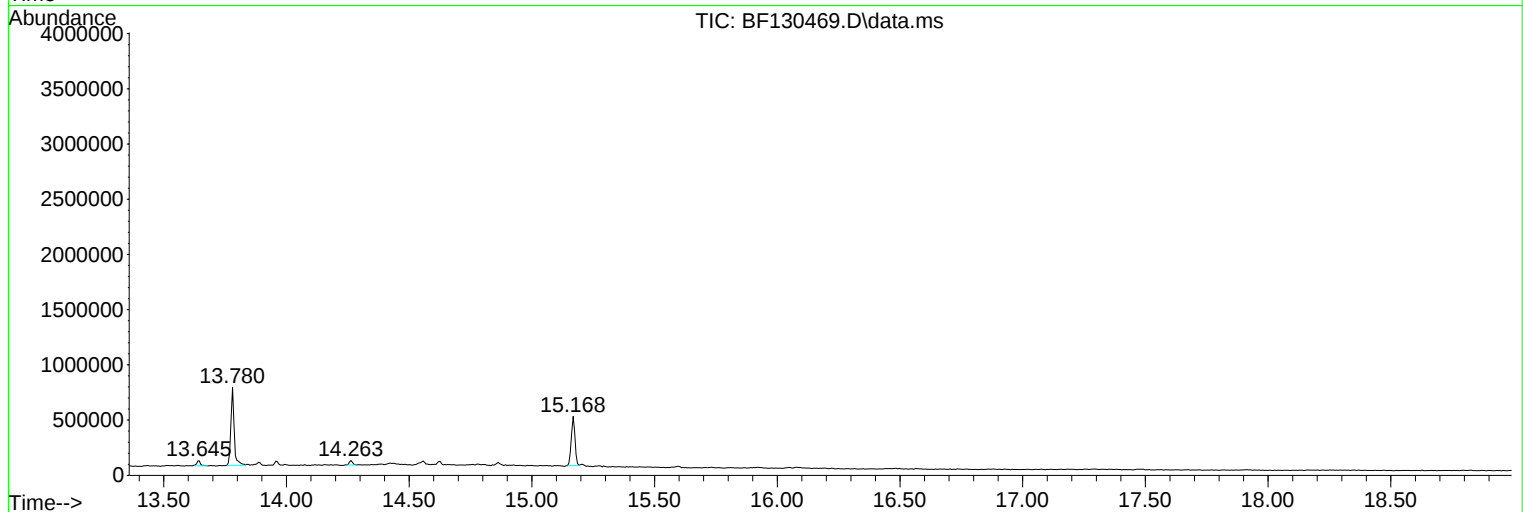
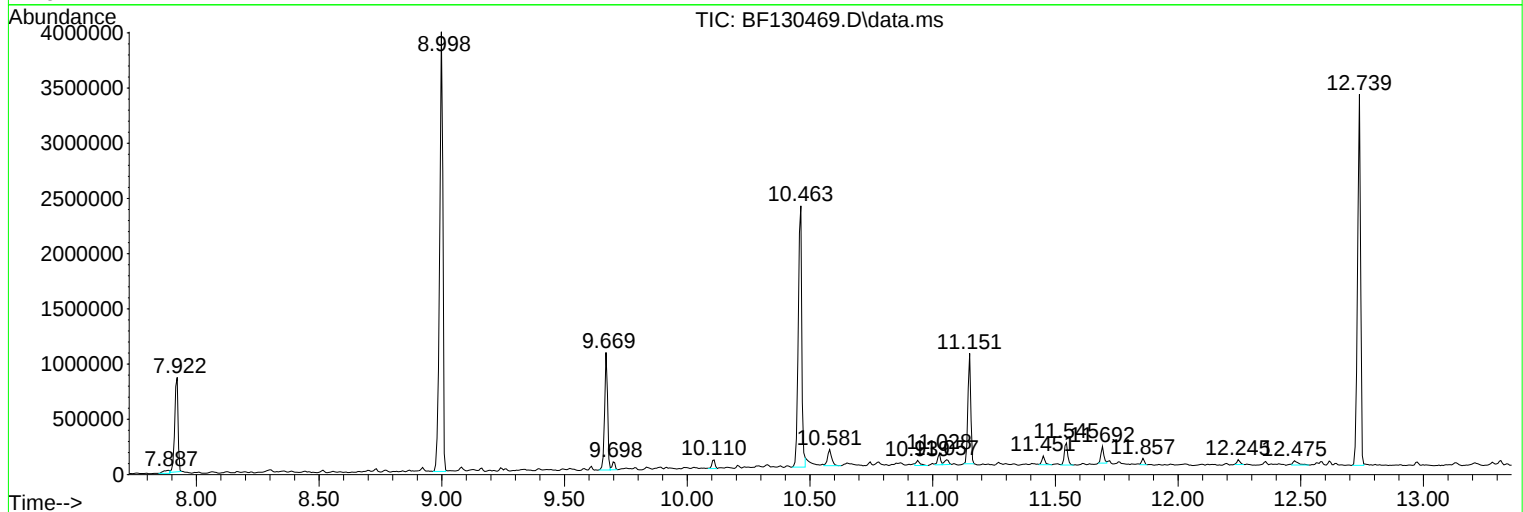
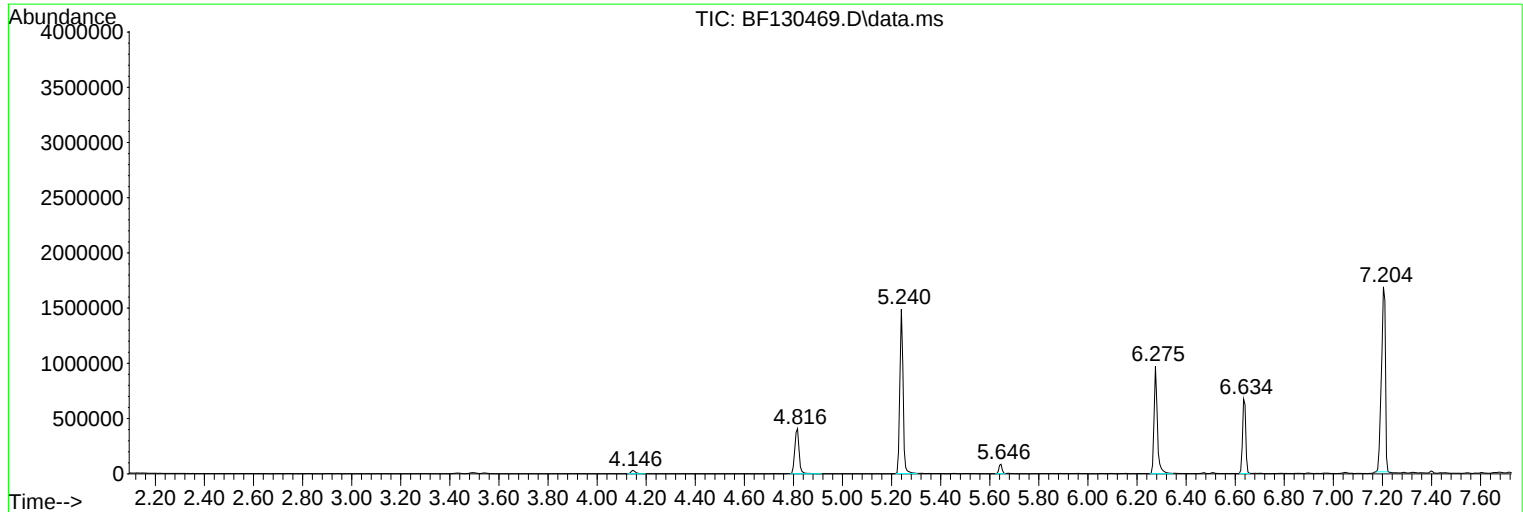
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ALS Vial : 9 Sample Multiplier: 1

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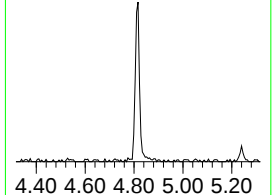
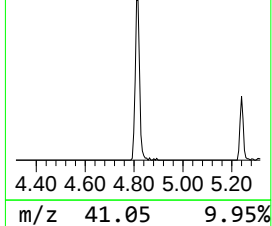
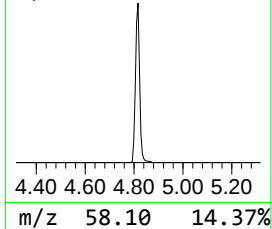
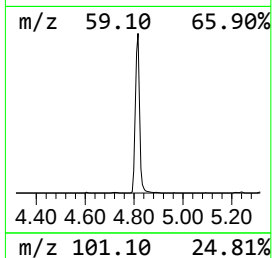
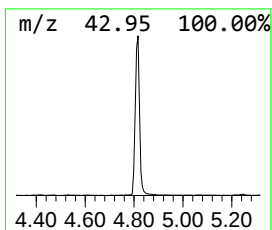
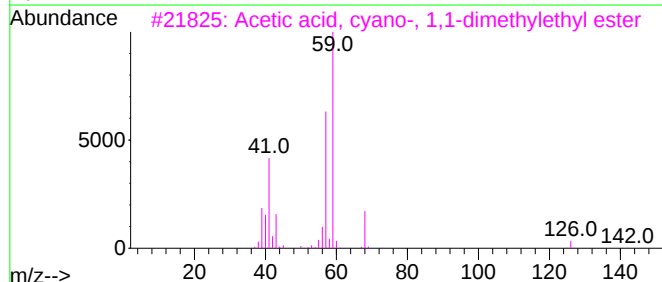
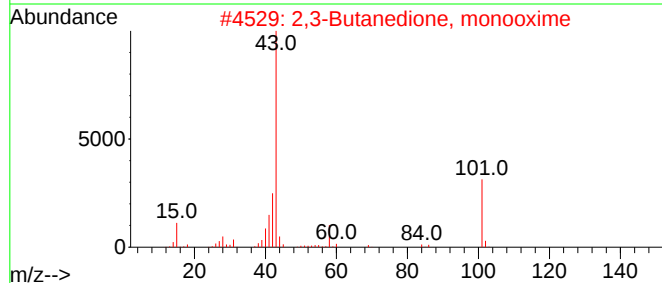
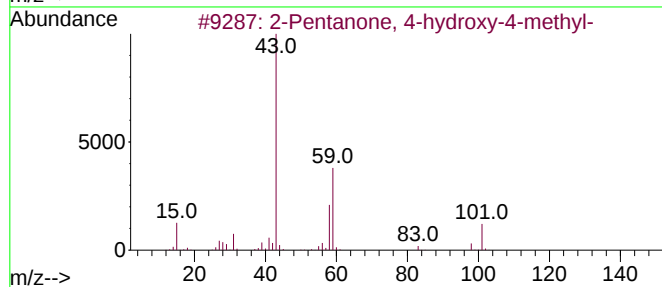
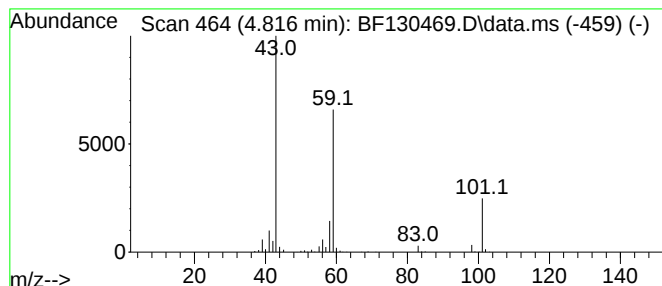
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.816	16.21 ng	497898	1,4-Dichlorobenzene-d4	6.634

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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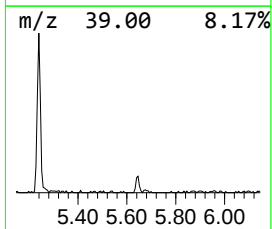
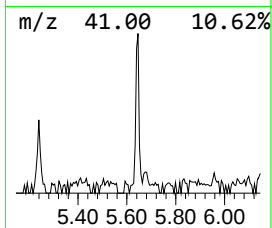
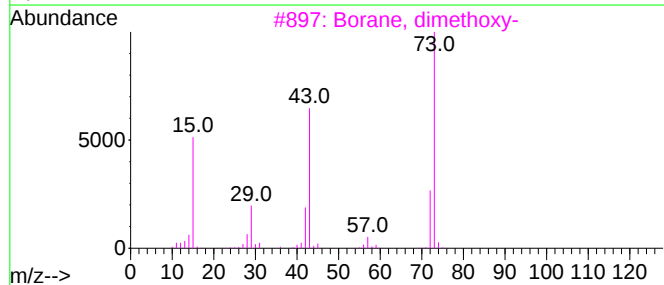
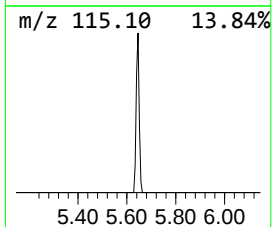
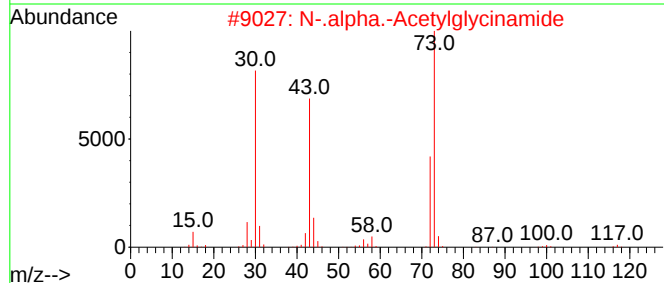
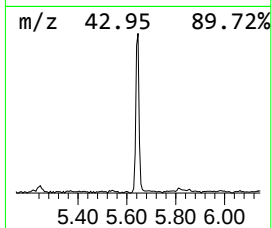
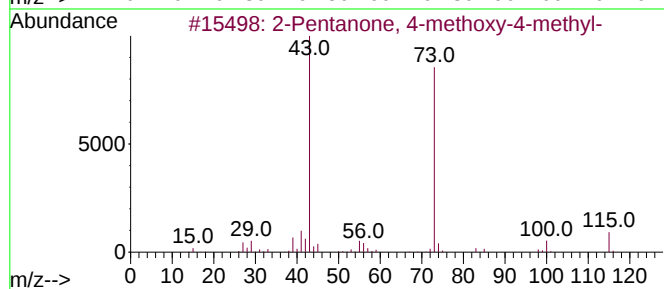
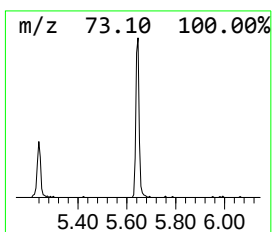
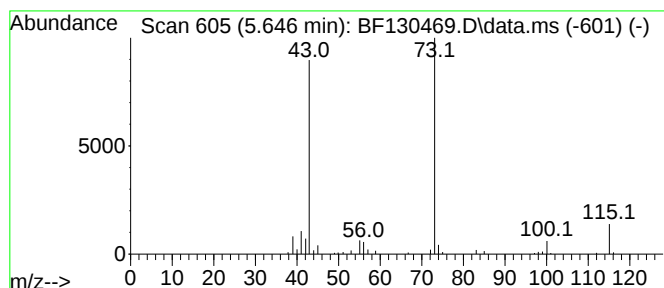
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.646	2.53 ng	77637	1,4-Dichlorobenzene-d4	6.634

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	43
3		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	33
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	10
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10



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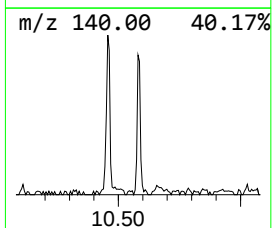
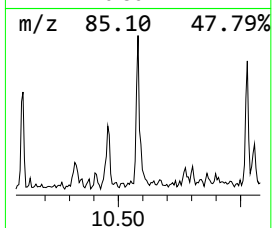
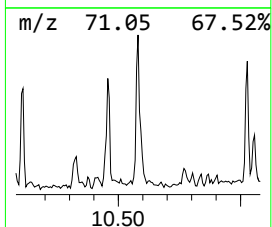
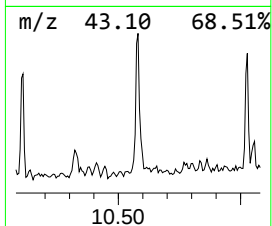
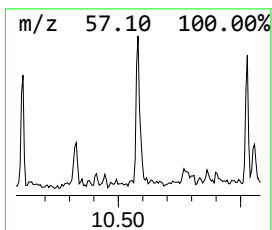
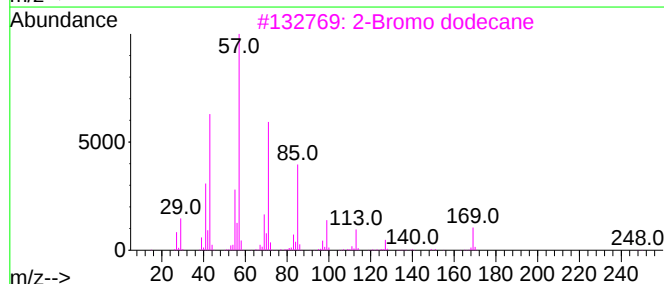
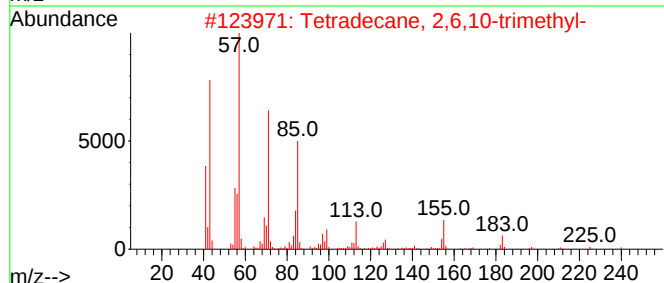
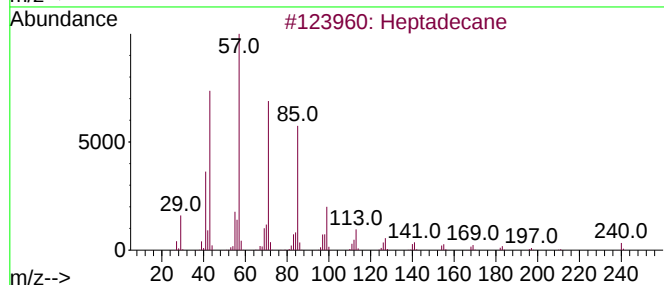
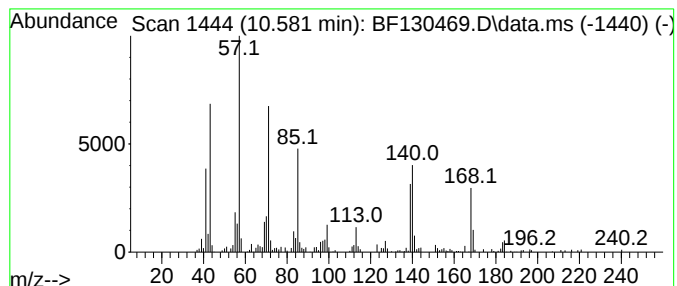
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.581	4.22 ng	171161	Phenanthrene-d10	11.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	89
2			Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	55
3			2-Bromo dodecane	248	C12H25Br	013187-99-0	53
4			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	49
5			Tetracosane	338	C24H50	000646-31-1	49



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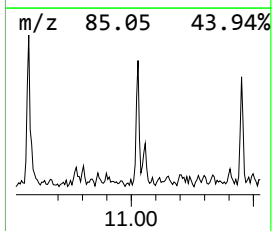
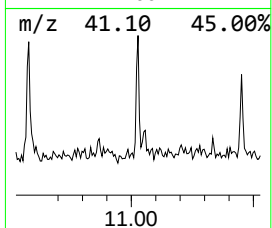
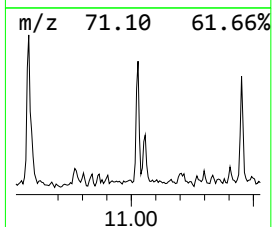
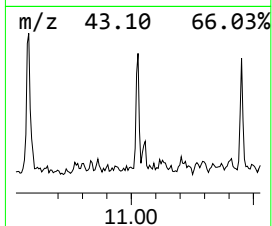
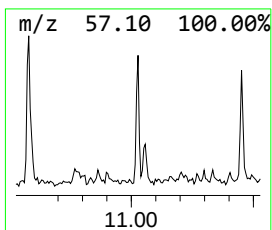
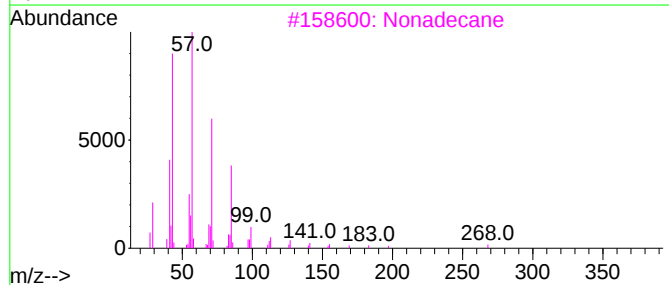
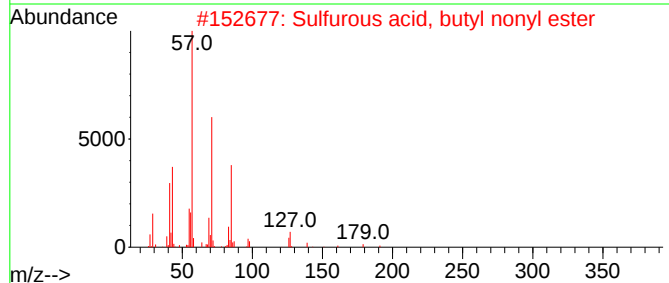
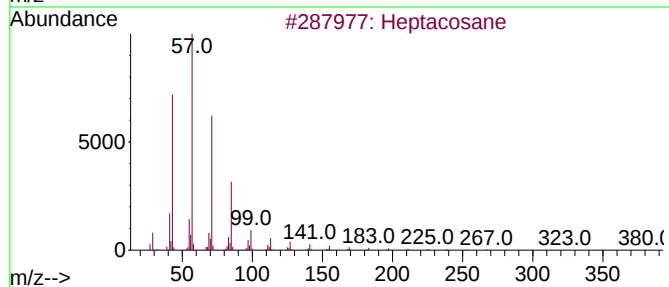
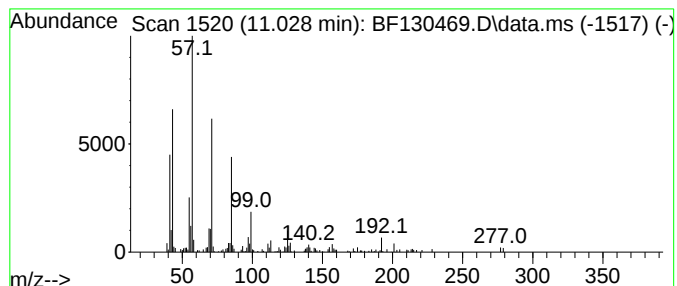
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Peak Number 4 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.028	2.03 ng	82204	Phenanthrene-d10	11.151

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	72
2		Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	59
3		Nonadecane	268	C19H40	000629-92-5	49
4		Octacosane	394	C28H58	000630-02-4	49
5		Tridecane	184	C13H28	000629-50-5	47



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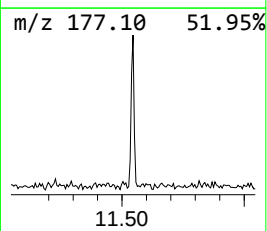
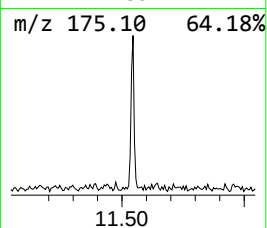
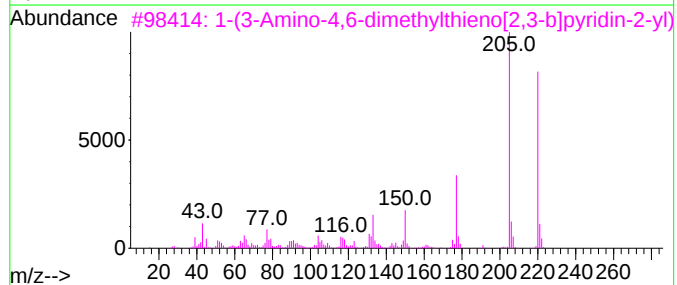
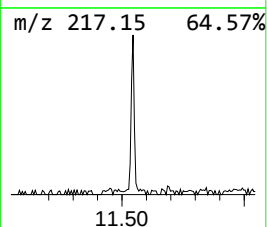
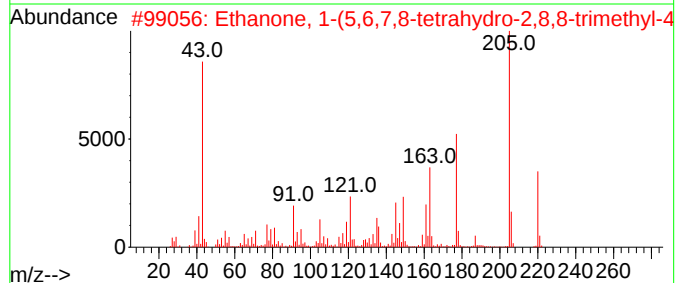
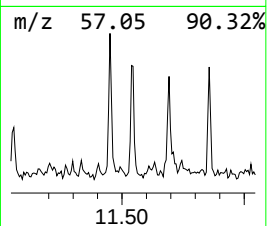
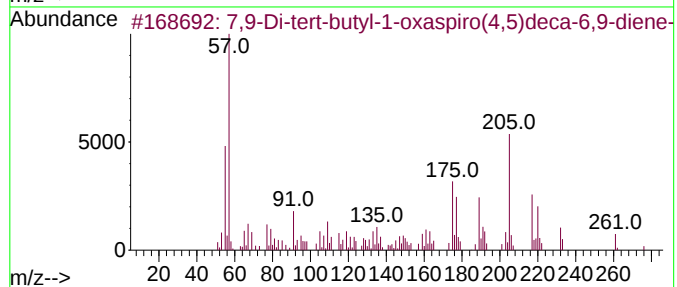
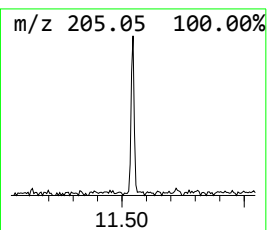
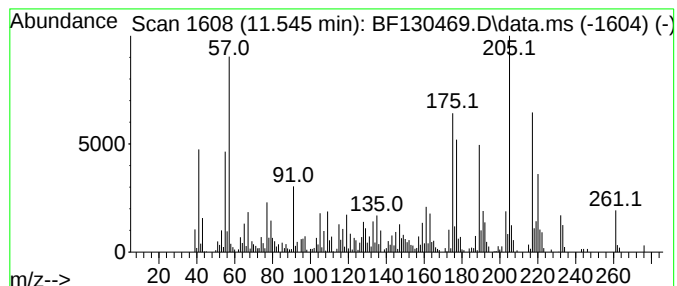
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.545	4.68 ng	189680	Phenanthrene-d10	11.151	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
3	1-(3-Amino-4,6-dimethylthieno[2,...	220	C11H12N2OS	052505-42-7	41
4	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
5	(1R,3aR,5aR,9aS)-1,4,4,7-Tetrame...	220	C15H24O	104188-25-2	25



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A2720

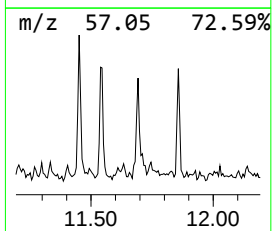
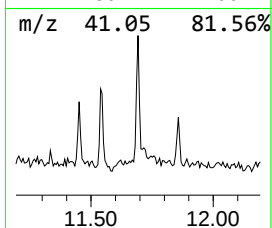
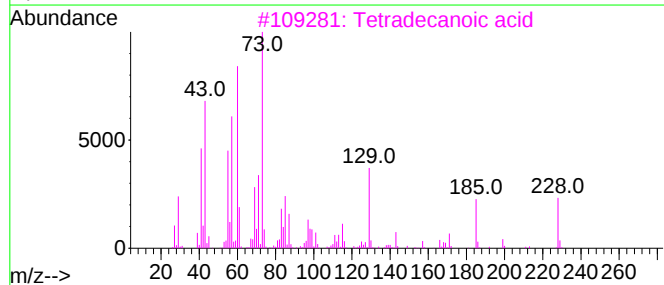
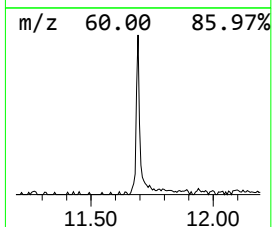
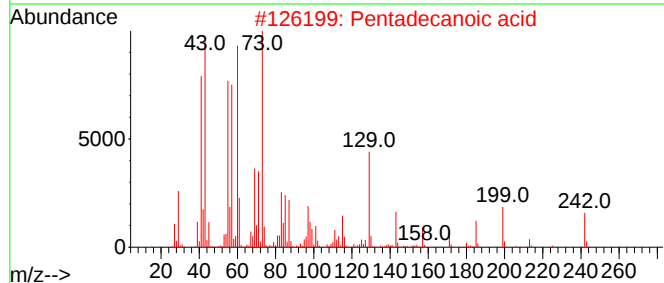
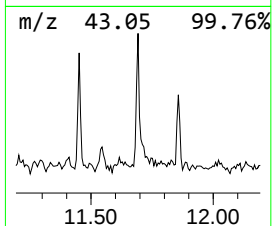
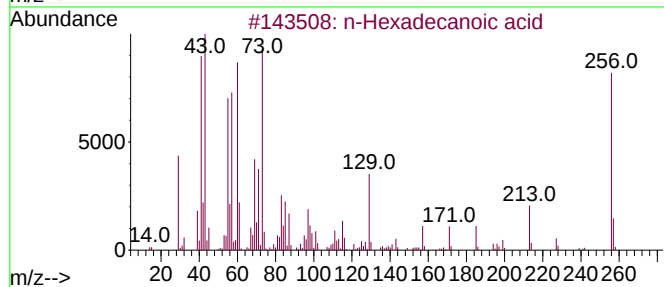
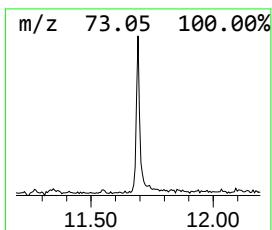
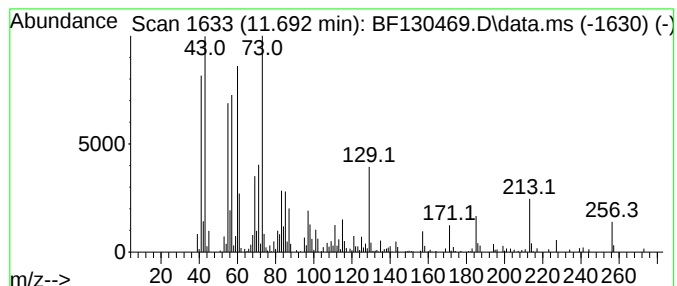
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.692	3.11 ng	126103	Phenanthrene-d10	11.151

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092922\
Data File : BF130469.D
Acq On : 29 Sep 2022 16:23
Operator : CG\JU
Sample : N4862-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
A2720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
2-Pentanone, 4-...	4.816	16.2	ng	497898	1	6.634	614344	20.0
2-Pentanone, 4-...	5.646	2.5	ng	77637	1	6.634	614344	20.0
Heptadecane	10.581	4.2	ng	171161	4	11.151	810250	20.0
Heptacosane	11.028	2.0	ng	82204	4	11.151	810250	20.0
7,9-Di-tert-but...	11.545	4.7	ng	189680	4	11.151	810250	20.0
n-Hexadecanoic ...	11.692	3.1	ng	126103	4	11.151	810250	20.0