

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
 Data File : BF132608.D
 Acq On : 02 Mar 2023 15:27
 Operator : CG\JU
 Sample : 01740-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-4-COMP-4

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.240	446	451	464	rVB	1537469	2023789	42.68%	5.117%
2	5.628	512	517	521	rBV	4228878	4224741	89.10%	10.682%
3	6.628	681	687	690	rBV	3939251	4215430	88.91%	10.658%
4	6.998	747	750	754	rVB	1506195	1183789	24.97%	2.993%
5	7.563	842	846	849	rBV	3073947	2800564	59.07%	7.081%
6	8.286	965	969	972	rBV	1912823	1570056	33.11%	3.970%
7	9.363	1147	1152	1155	rBV	5398246	4741335	100.00%	11.988%
8	10.045	1265	1268	1271	rBV	2088006	1788738	37.73%	4.523%
9	10.080	1271	1274	1277	rVB	125388	101026	2.13%	0.255%
10	10.251	1300	1303	1306	rBV	66345	60168	1.27%	0.152%
11	10.598	1358	1362	1365	rBV	89905	76384	1.61%	0.193%
12	10.763	1386	1390	1393	rVB	473306	385761	8.14%	0.975%
13	10.845	1399	1404	1407	rBV	3328907	3318971	70.00%	8.392%
14	11.545	1519	1523	1525	rBV	2206775	1919264	40.48%	4.853%
15	11.569	1525	1527	1530	rVV	615087	476770	10.06%	1.205%
16	11.616	1530	1535	1538	rVV2	131450	182143	3.84%	0.461%
17	11.774	1557	1562	1565	rBV2	72232	77956	1.64%	0.197%
18	12.063	1602	1611	1619	rBV3	562119	1020755	21.53%	2.581%
19	12.163	1625	1628	1630	rBV2	76212	68255	1.44%	0.173%
20	12.492	1680	1684	1686	rBV2	77296	78370	1.65%	0.198%
21	12.763	1727	1730	1734	rBV	534806	499305	10.53%	1.262%
22	12.851	1742	1745	1754	rBV	179499	315854	6.66%	0.799%
23	12.998	1763	1770	1773	rBV	429485	471574	9.95%	1.192%
24	13.139	1789	1794	1797	rBV	4595611	4341494	91.57%	10.977%
25	13.510	1851	1857	1863	rVB2	133486	155902	3.29%	0.394%
26	14.039	1938	1947	1960	rBV5	212942	717753	15.14%	1.815%
27	14.204	1970	1975	1978	rBV	1142719	1113424	23.48%	2.815%
28	14.227	1978	1979	1986	rVB	123796	95508	2.01%	0.241%
29	14.962	2099	2104	2114	rVB3	106982	281247	5.93%	0.711%
30	15.686	2224	2227	2233	rVB	77161	102676	2.17%	0.260%
31	15.757	2234	2239	2249	rVB	861908	1142348	24.09%	2.888%

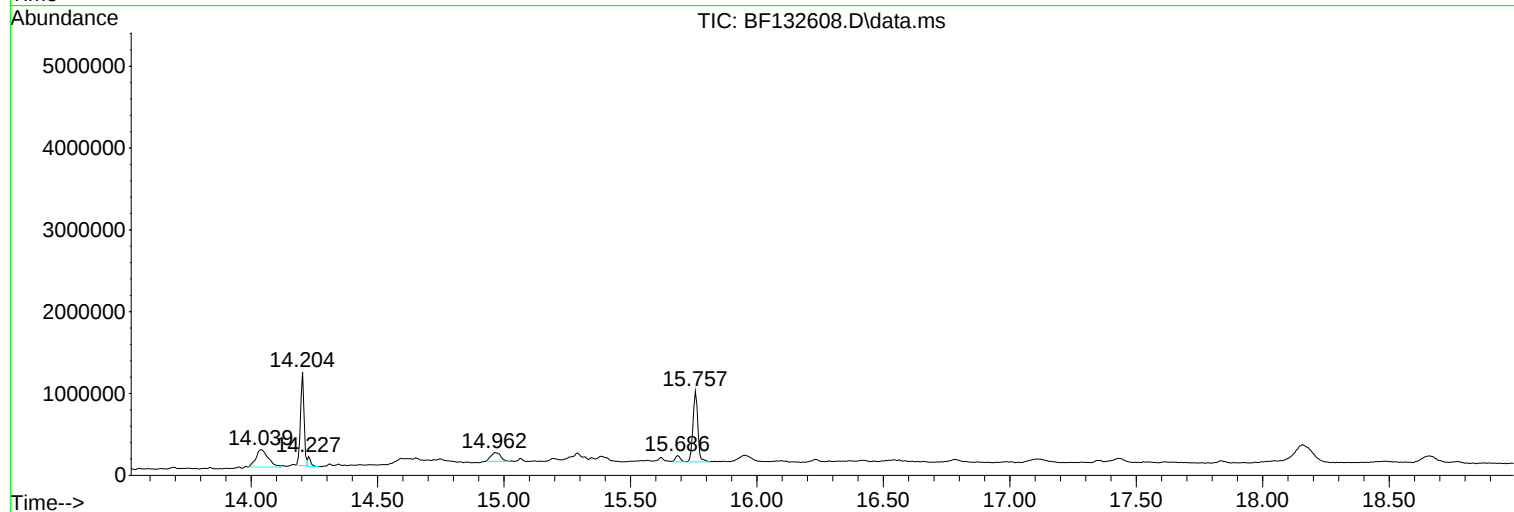
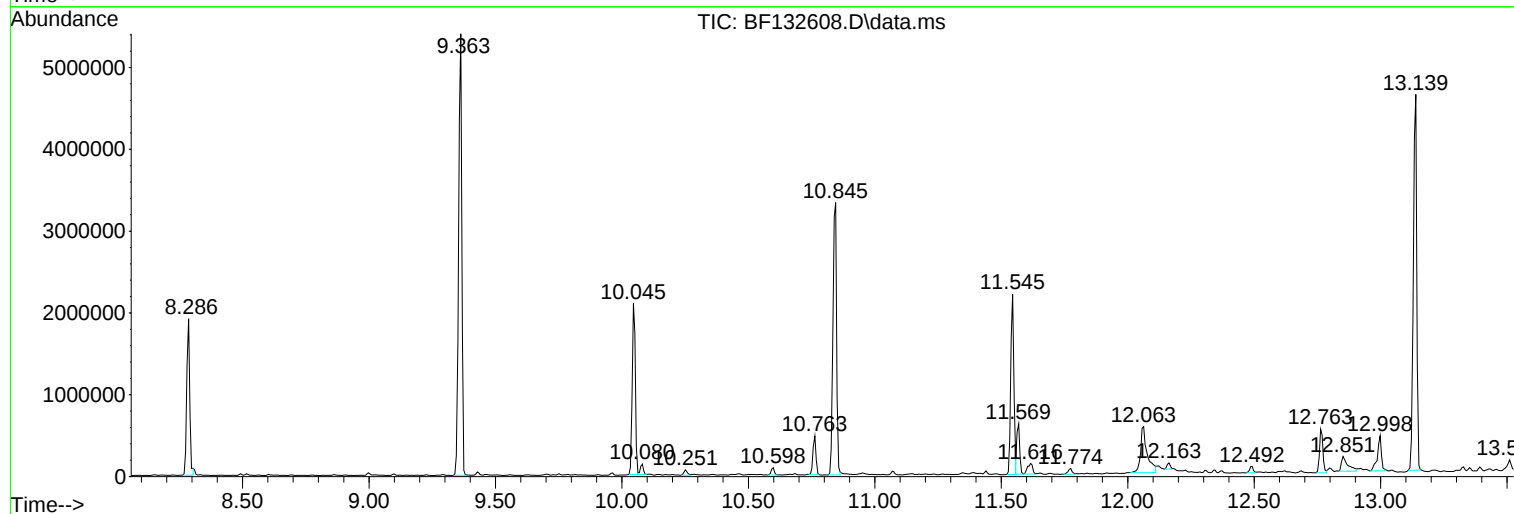
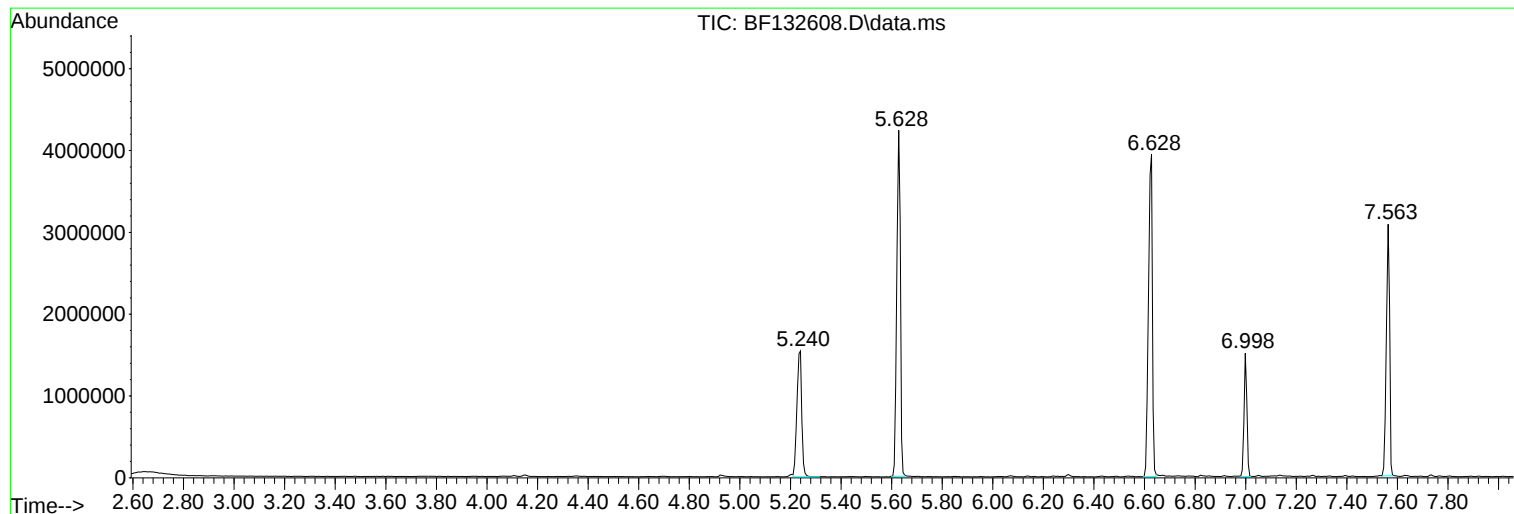
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ClientSampleId :
SAMPLE-4-COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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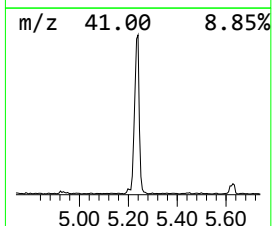
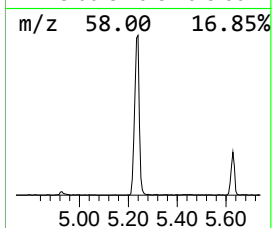
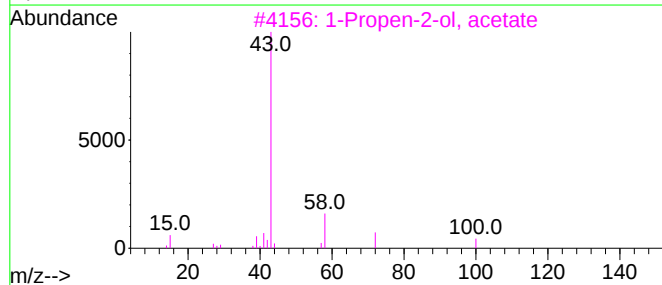
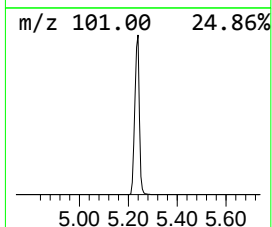
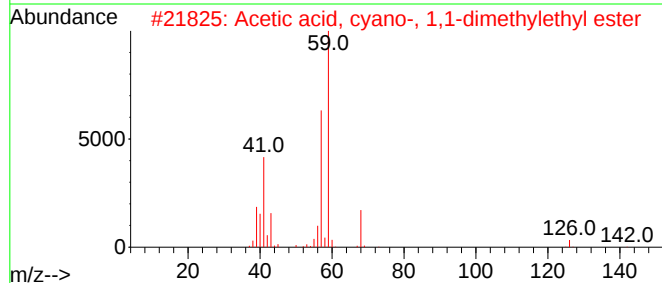
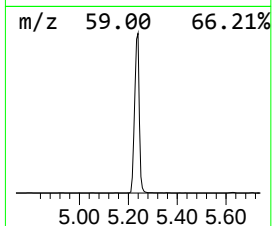
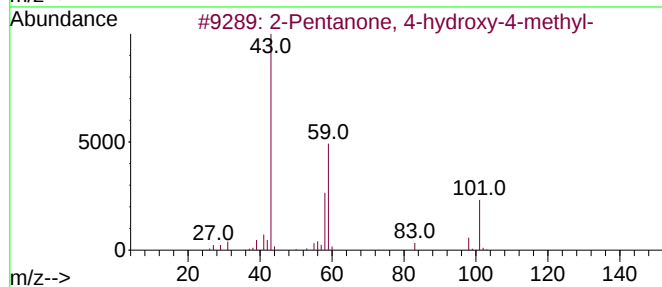
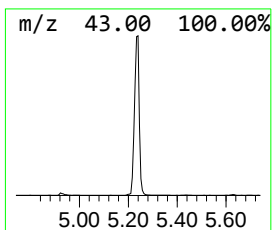
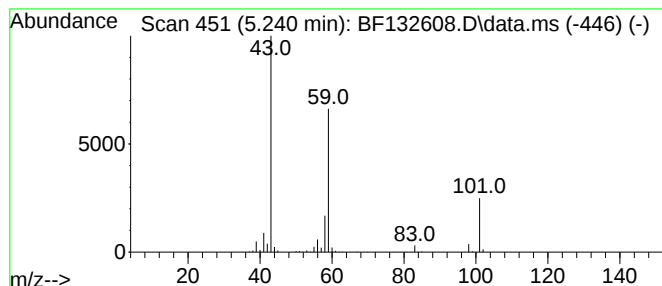
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.240	34.19 ng	2023790	1,4-Dichlorobenzene-d4	6.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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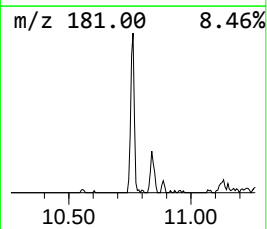
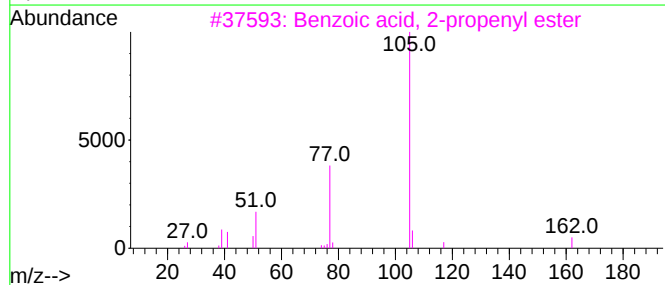
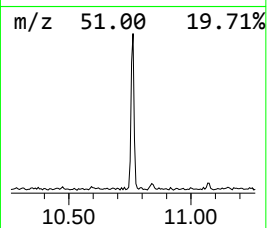
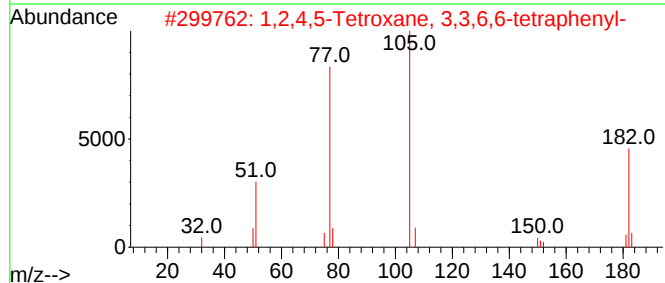
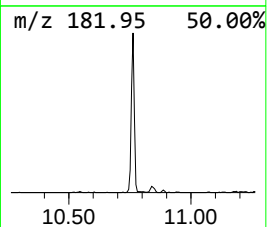
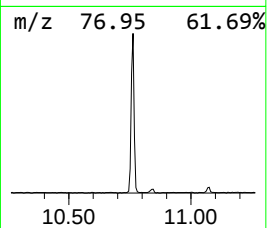
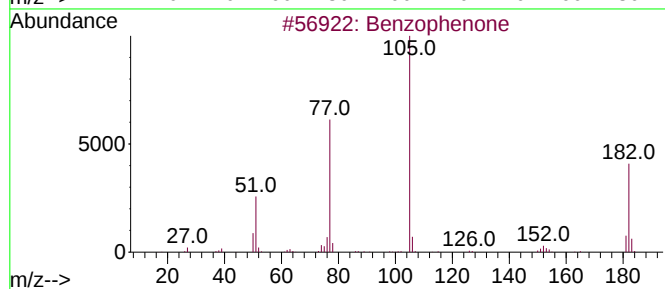
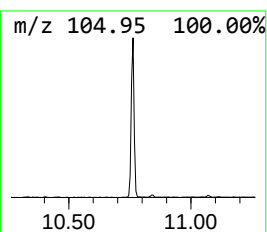
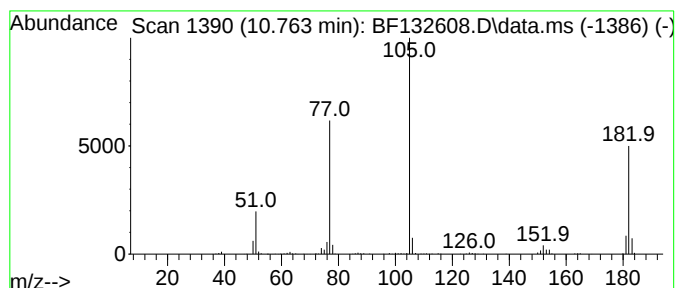
Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-COMP-4

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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.763	4.31 ng	385761	Acenaphthene-d10	10.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
4	2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



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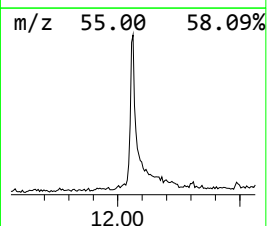
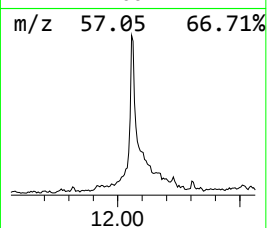
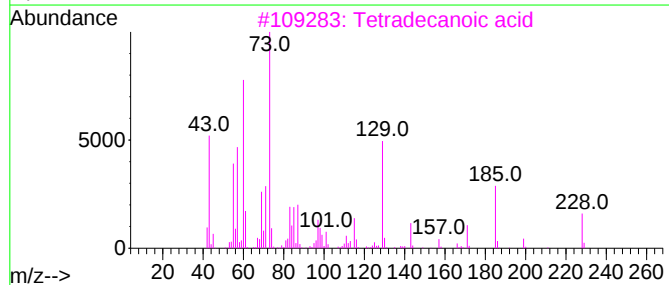
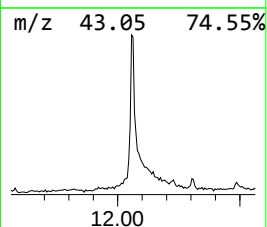
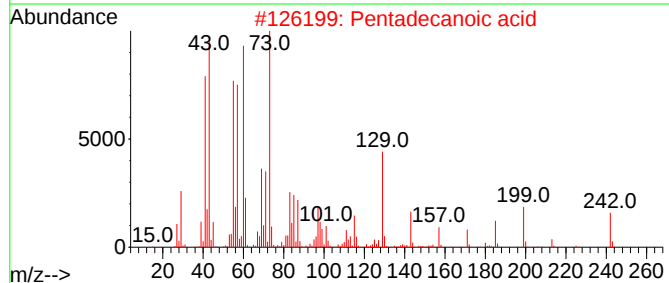
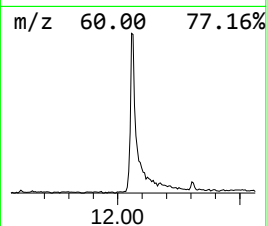
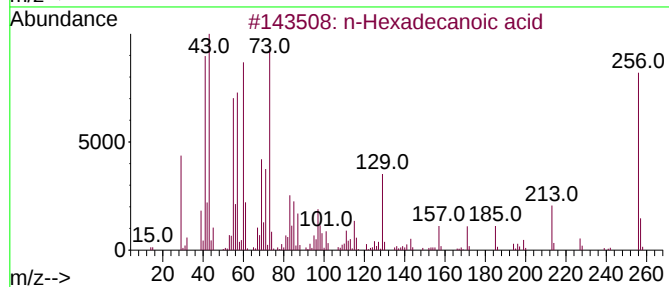
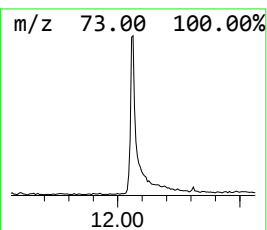
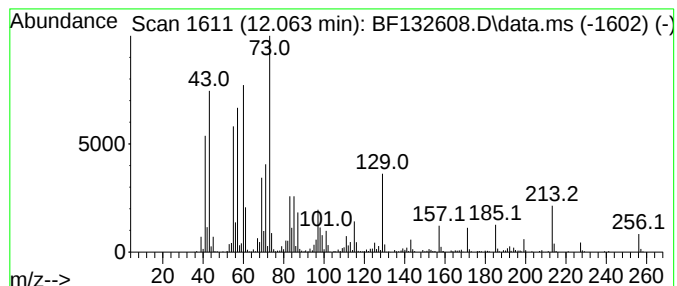
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.063	10.64 ng	1020760	Phenanthrene-d10		11.545	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
4	Dodecanoic acid		200	C12H24O2	000143-07-7	64
5	Tridecanoic acid		214	C13H26O2	000638-53-9	64



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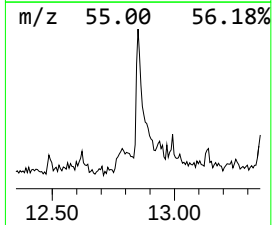
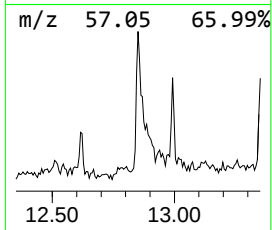
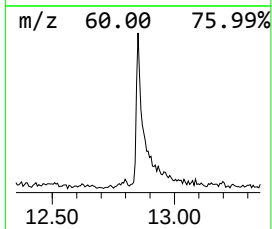
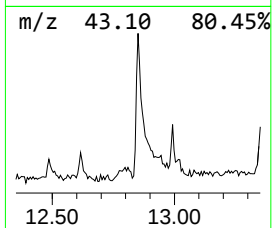
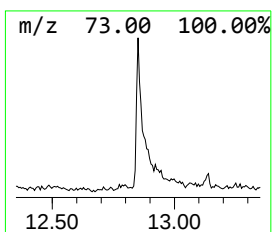
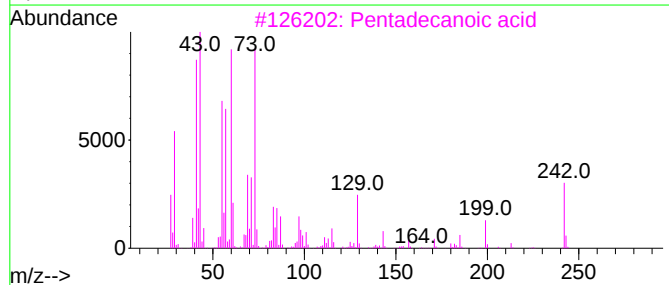
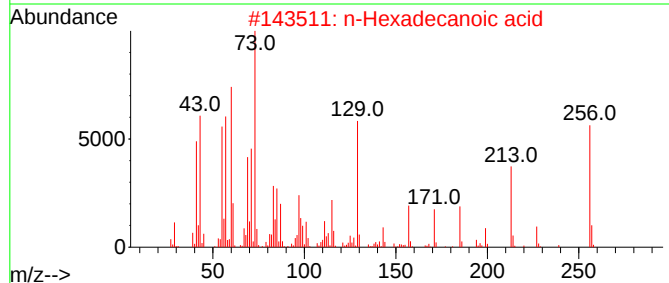
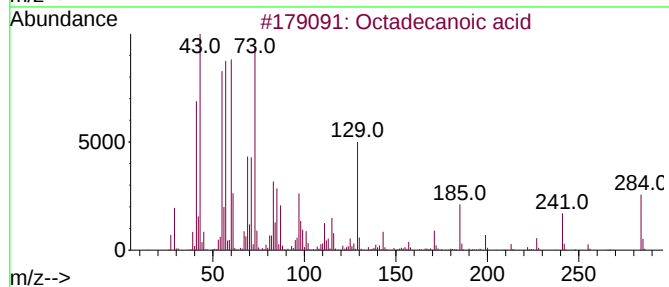
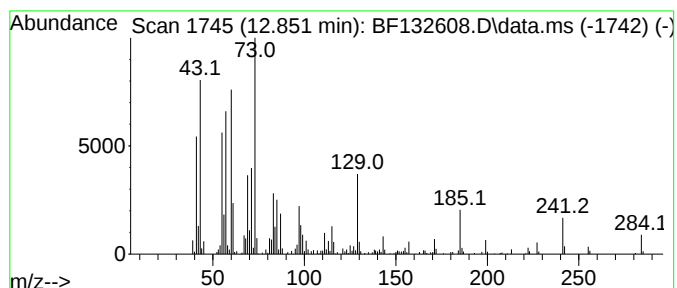
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.851	3.29 ng	315854	Phenanthrene-d10	11.545	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	90



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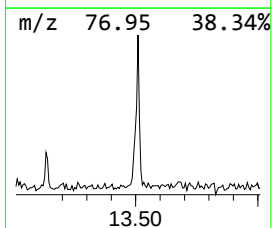
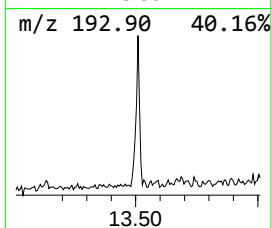
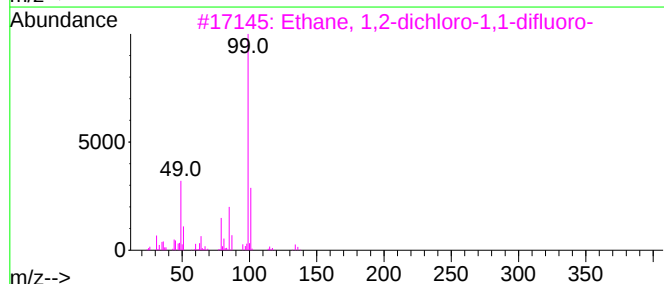
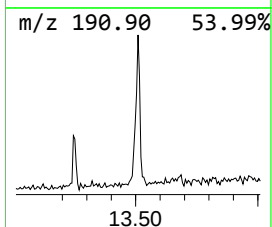
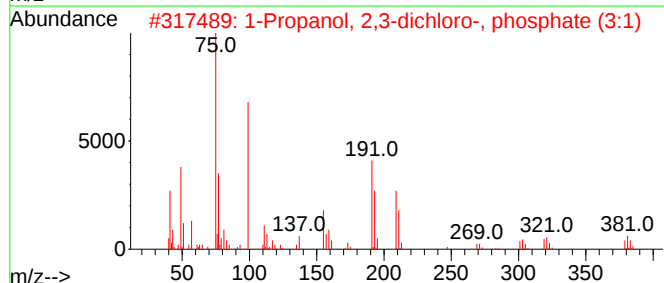
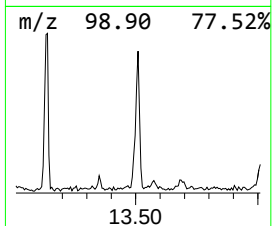
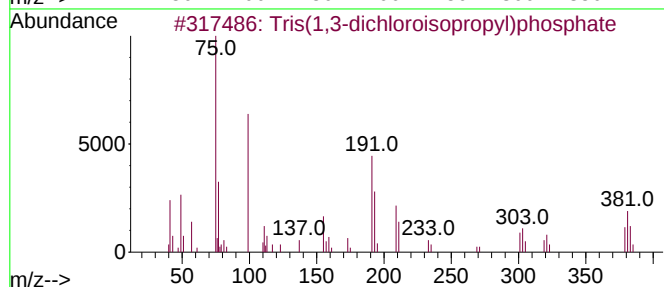
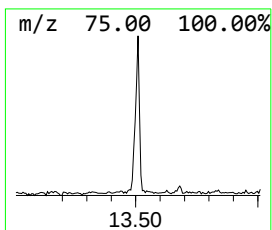
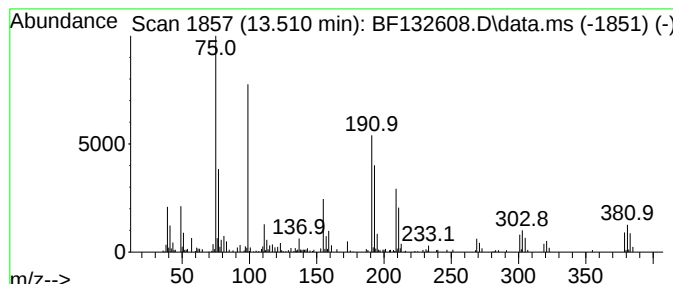
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tris(1,3-dichloroisopropyl)... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	2.80 ng	155902	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tris(1,3-dichloroisopropyl)phosp...	428	C9H15Cl6O4P	013674-87-8	91
2			1-Propanol, 2,3-dichloro-, phosph...	428	C9H15Cl6O4P	000078-43-3	49
3			Ethane, 1,2-dichloro-1,1-difluoro-	134	C2H2Cl2F2	001649-08-7	27
4			1-Propene, 1,3-dichloro-, (E)-	110	C3H4Cl2	010061-02-6	16
5			1-Propene, 1,3-dichloro-, (Z)-	110	C3H4Cl2	010061-01-5	12



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Misc :
ALS Vial : 5 Sample Multiplier: 1

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ClientSampleId :
SAMPLE-4-COMP-4

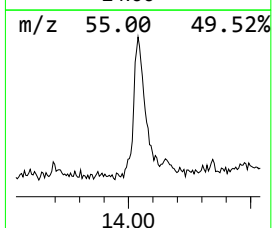
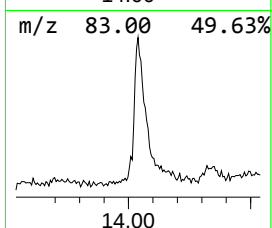
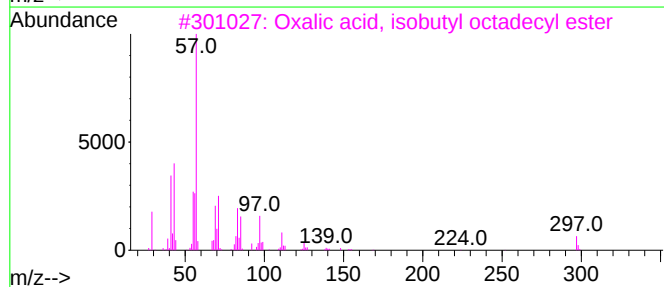
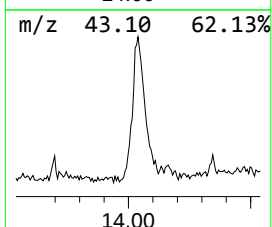
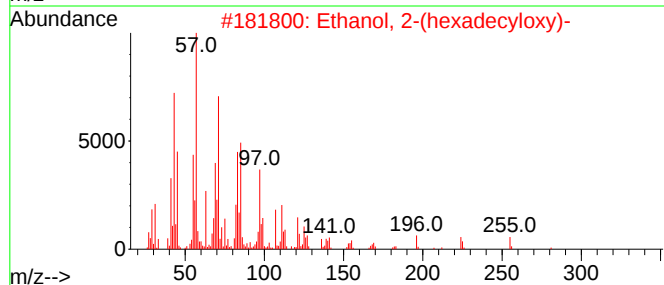
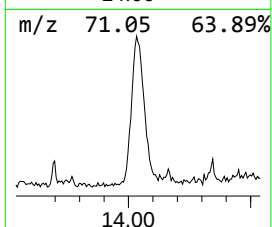
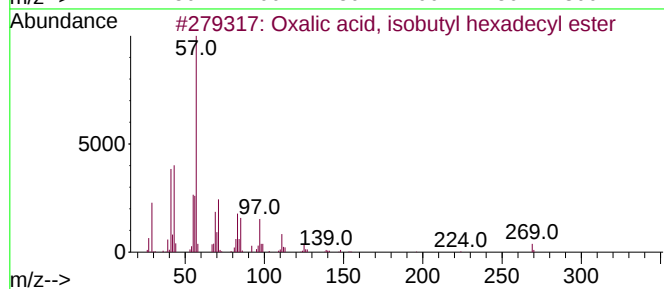
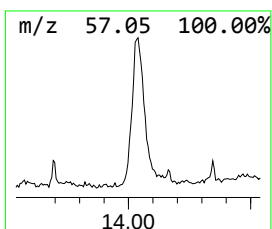
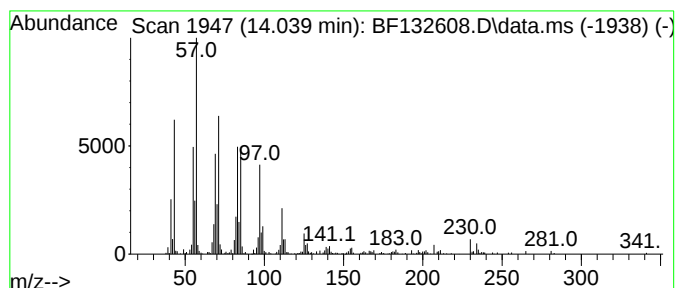
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxalic acid, isobutyl hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.039	12.89 ng	717753	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91
3			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
4			Carbonic acid, decyl octadecyl e...	454	C29H58O3	1000383-16-7	91
5			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132608.D
Acq On : 02 Mar 2023 15:27
Operator : CG\JU
Sample : 01740-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-COMP-4

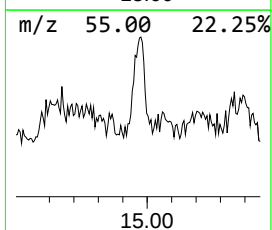
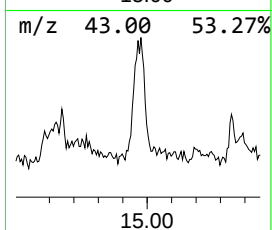
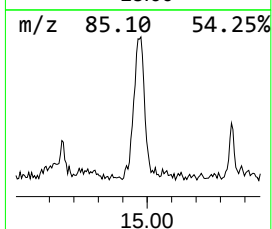
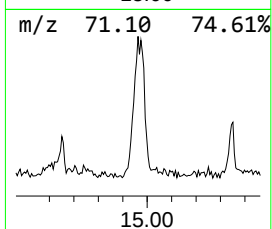
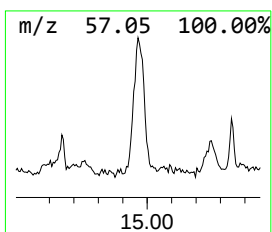
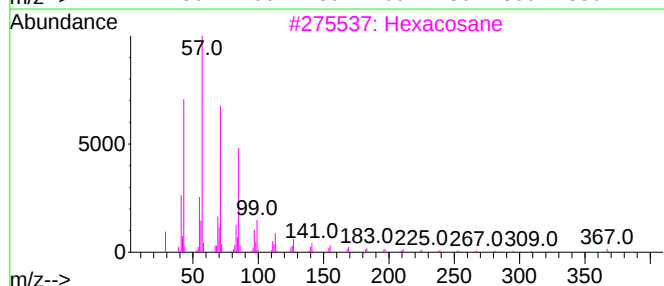
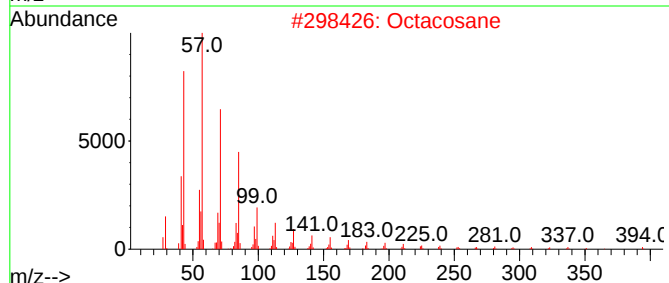
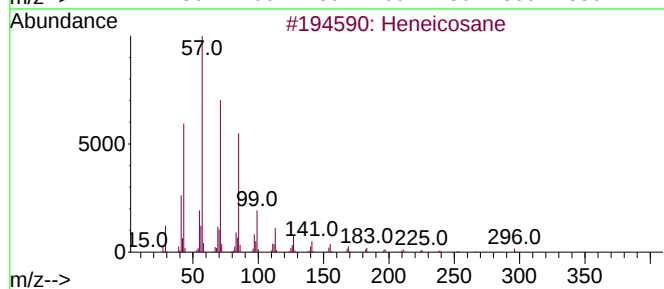
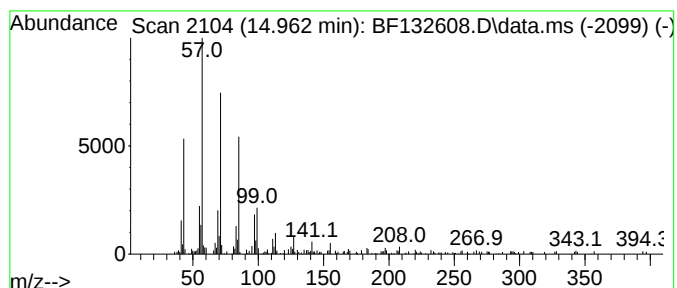
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.963	5.05 ng	281247	Chrysene-d12	14.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	96
2			Octacosane	394	C28H58	000630-02-4	93
3			Hexacosane	366	C26H54	000630-01-3	87
4			Tetracosane	338	C24H50	000646-31-1	86
5			Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
Data File : BF132608.D
Acq On : 02 Mar 2023 15:27
Operator : CG\JU
Sample : 01740-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAMPLE-4-COMP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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-...	5.240	34.2	ng	2023790	1	6.998	1183790	20.0
Benzophenone	10.763	4.3	ng	385761	3	10.045	1788740	20.0
n-Hexadecanoic ...	12.063	10.6	ng	1020760	4	11.545	1919260	20.0
Octadecanoic acid	12.851	3.3	ng	315854	4	11.545	1919260	20.0
Tris(1,3-dichlo...	13.510	2.8	ng	155902	5	14.204	1113420	20.0
Oxalic acid, is...	14.039	12.9	ng	717753	5	14.204	1113420	20.0
Heneicosane	14.963	5.0	ng	281247	5	14.204	1113420	20.0