

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
 Data File : BF132714.D
 Acq On : 09 Mar 2023 12:57
 Operator : CG\JU
 Sample : 01829-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SS-02-20230306

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: BF132714.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.204	441	445	456	rVB	1337050	1588787	41.90%	5.553%
2	5.610	510	514	530	rVB	3409473	3171593	83.65%	11.085%
3	6.610	680	684	687	rBV	3523832	3146662	82.99%	10.998%
4	6.804	714	717	722	rBV	43371	49981	1.32%	0.175%
5	6.981	743	747	750	rBV	1323572	1086731	28.66%	3.798%
6	7.540	838	842	846	rBV	2255147	2090505	55.13%	7.307%
7	8.263	961	965	968	rBV	1790947	1387139	36.58%	4.848%
8	9.339	1144	1148	1151	rBV	4699097	3791712	100.00%	13.253%
9	10.028	1261	1265	1268	rBV	1680247	1523892	40.19%	5.326%
10	10.739	1382	1386	1389	rVB	755567	651551	17.18%	2.277%
11	10.816	1395	1399	1403	rBV	2193921	1972037	52.01%	6.893%
12	11.369	1489	1493	1496	rBV	145179	120716	3.18%	0.422%
13	11.427	1500	1503	1506	rBV	54119	45899	1.21%	0.160%
14	11.522	1515	1519	1522	rBV	1551338	1308874	34.52%	4.575%
15	12.033	1602	1606	1610	rBV	301360	331981	8.76%	1.160%
16	12.745	1722	1727	1731	rBV5	33184	62843	1.66%	0.220%
17	12.822	1737	1740	1750	rBV	90696	135657	3.58%	0.474%
18	12.969	1762	1765	1767	rBV2	78045	85256	2.25%	0.298%
19	12.992	1767	1769	1774	rVB	63696	57331	1.51%	0.200%
20	13.110	1785	1789	1792	rBV	3490330	2973957	78.43%	10.394%
21	13.580	1866	1869	1874	rVB	77891	65602	1.73%	0.229%
22	13.998	1937	1940	1949	rBV	284588	409802	10.81%	1.432%
23	14.139	1961	1964	1967	rBV	125063	122130	3.22%	0.427%
24	14.180	1967	1971	1974	rBV	1292403	1115246	29.41%	3.898%
25	14.268	1983	1986	1991	rBV	228239	218710	5.77%	0.764%
26	14.798	2074	2076	2080	rVB	82920	75747	2.00%	0.265%
27	15.721	2229	2233	2239	rVB	766497	1020677	26.92%	3.567%

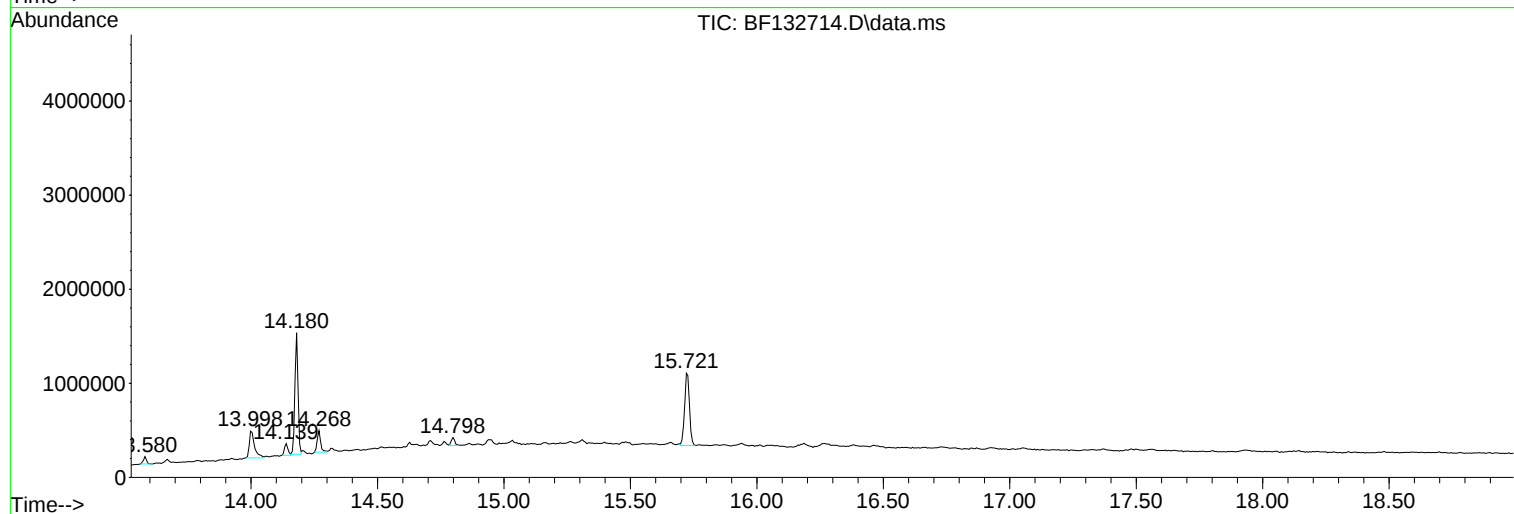
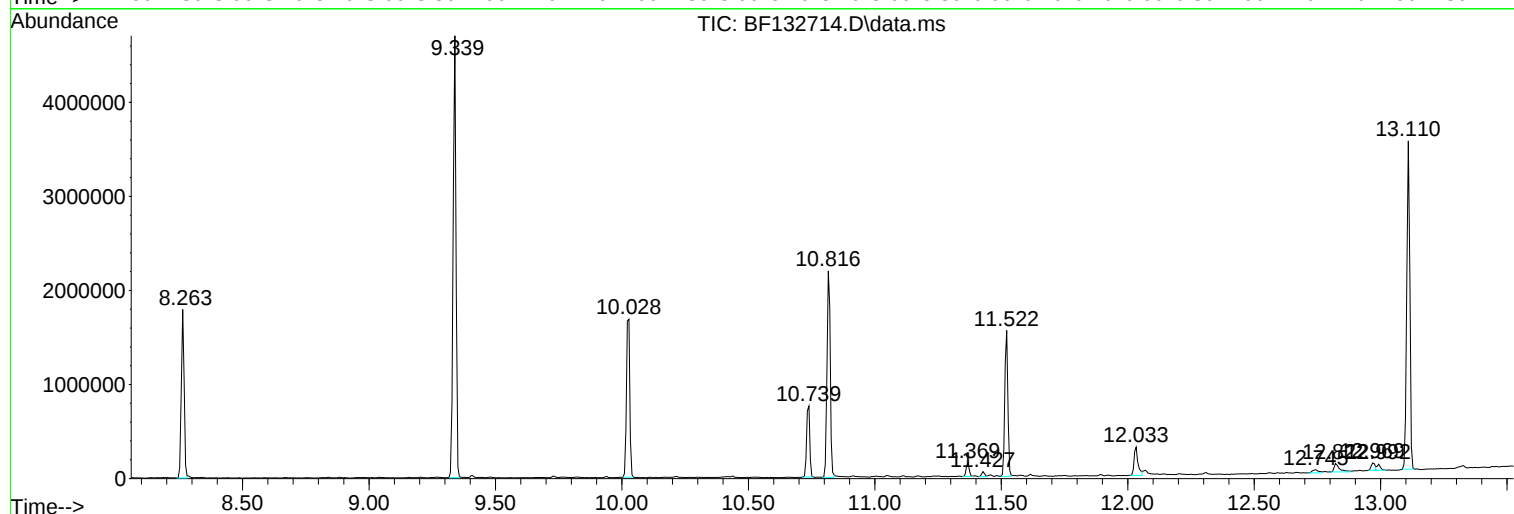
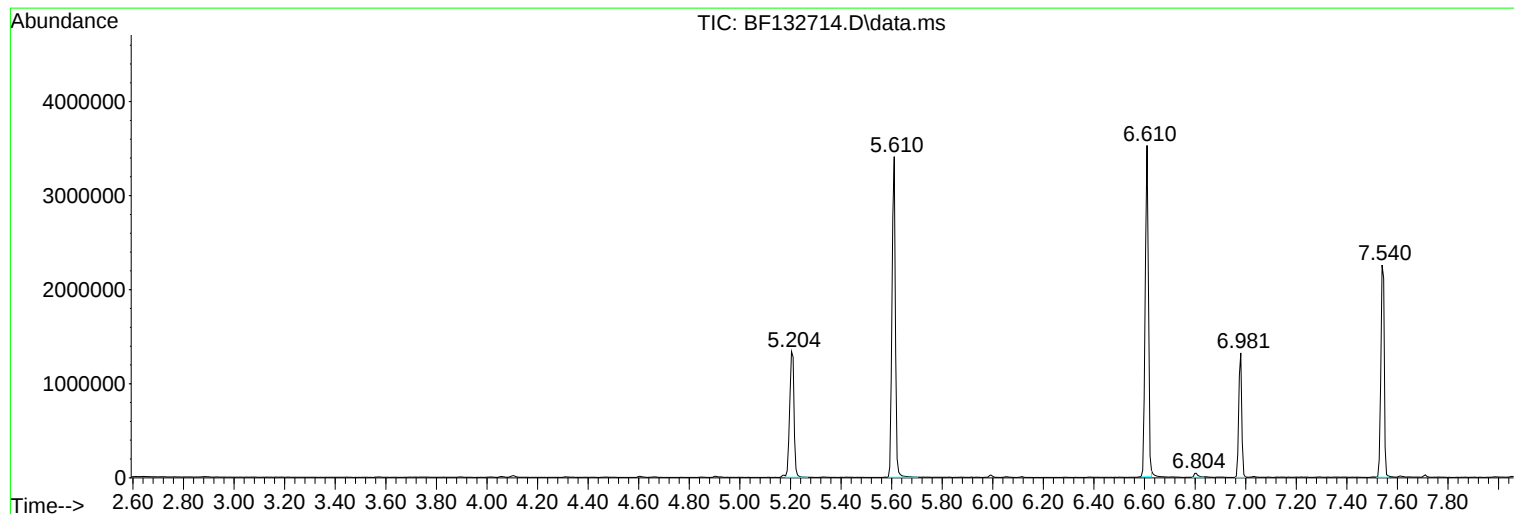
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Instrument :
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ClientSampleId :
SS-02-20230306

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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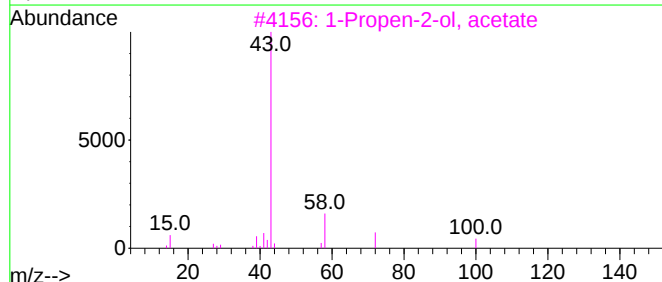
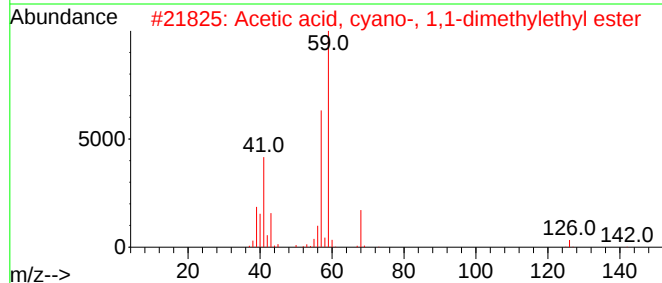
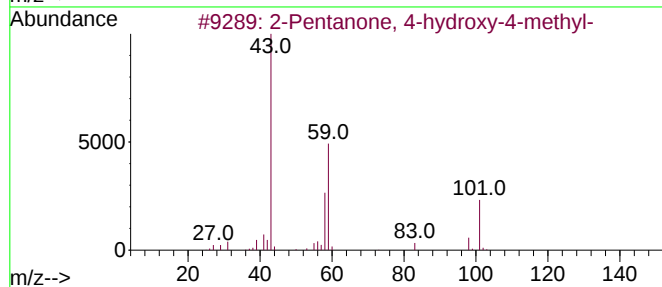
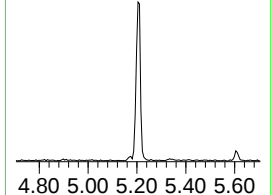
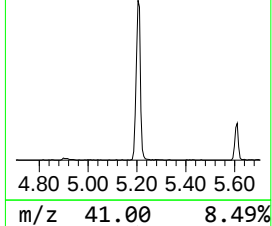
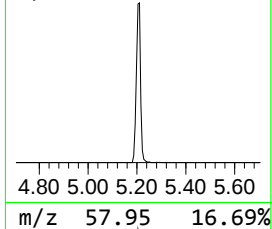
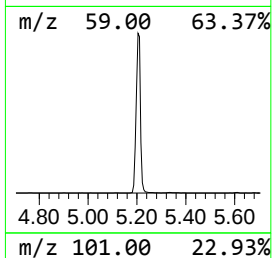
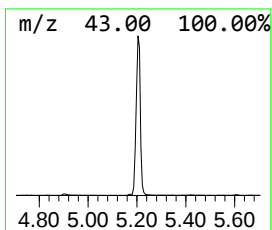
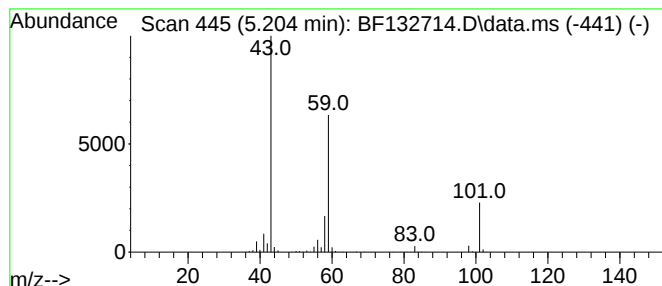
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.204	29.24 ng	1588790	1,4-Dichlorobenzene-d4	6.981

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			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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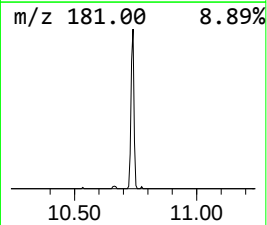
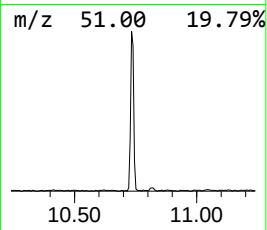
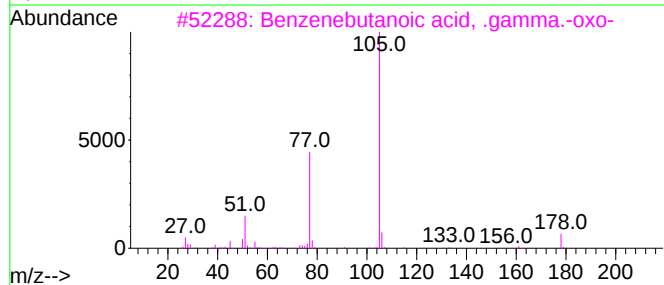
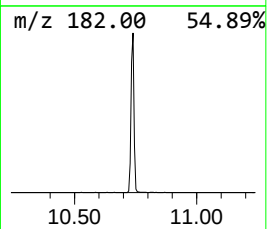
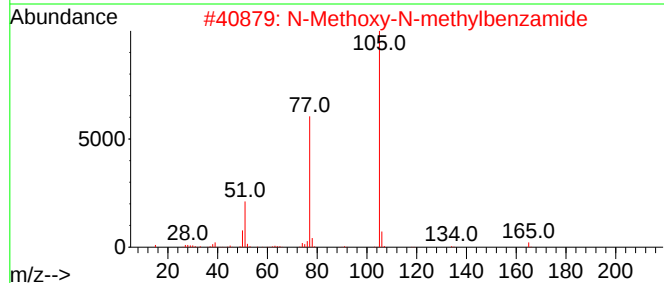
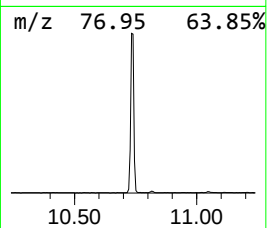
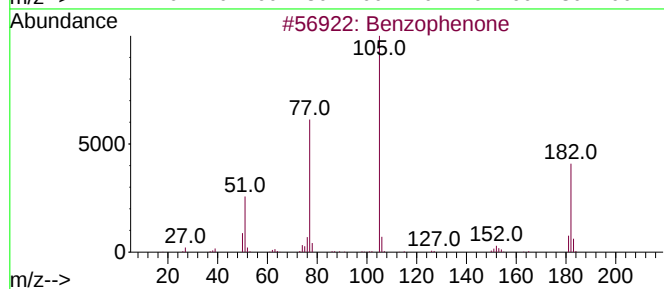
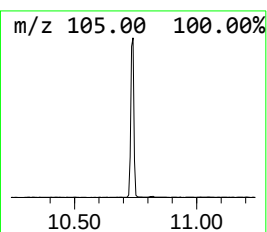
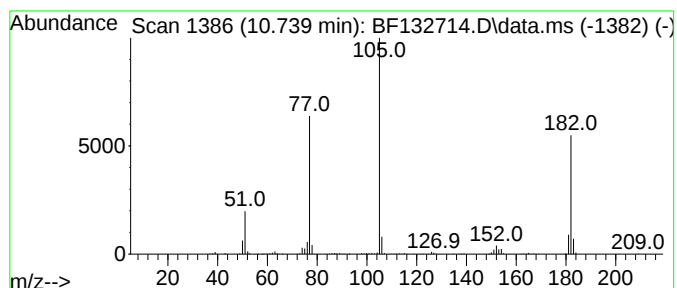
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	8.55 ng	651551	Acenaphthene-d10	10.028

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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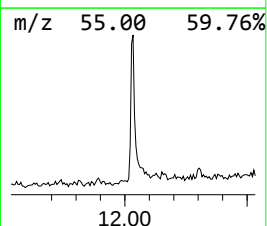
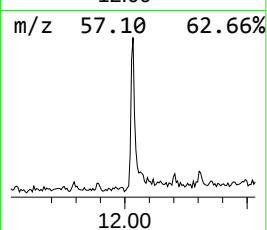
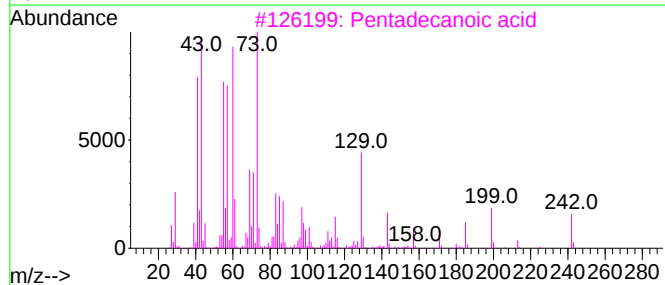
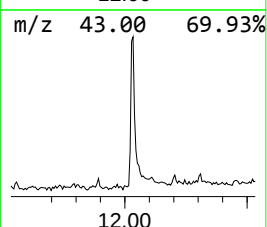
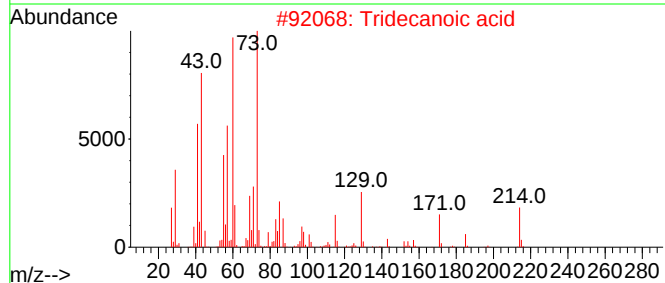
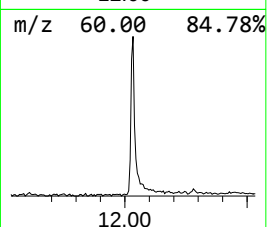
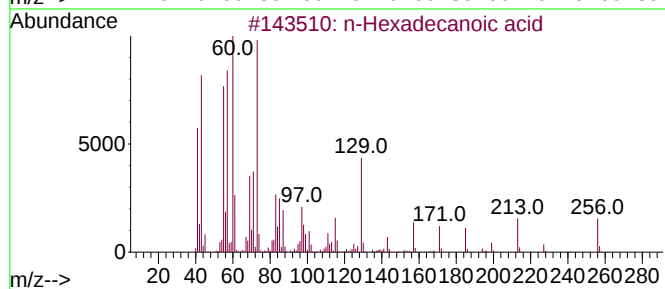
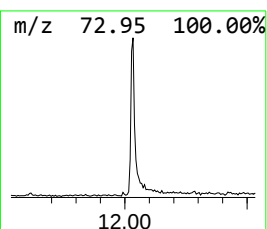
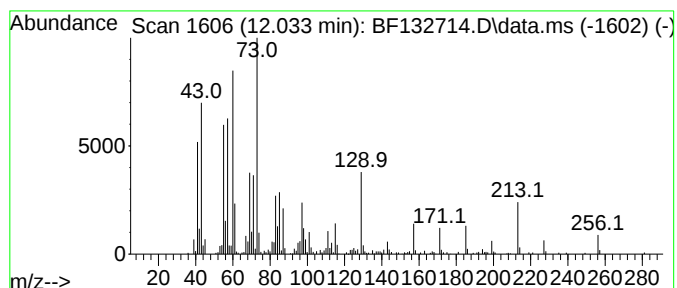
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.033	5.07 ng	331981	Phenanthrene-d10	11.522	
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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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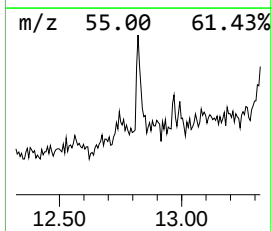
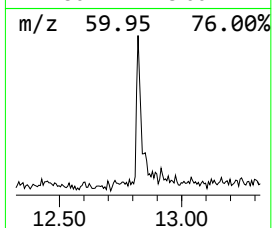
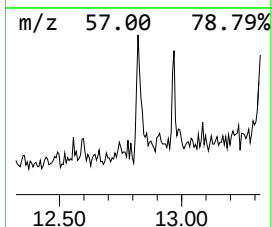
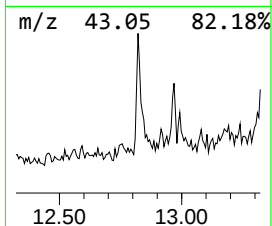
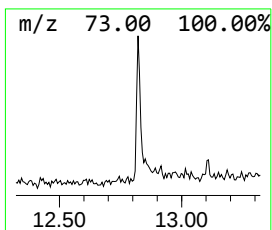
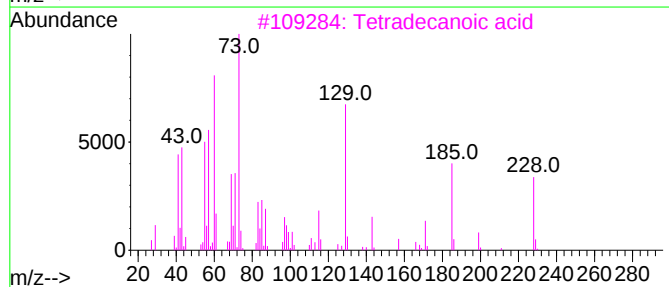
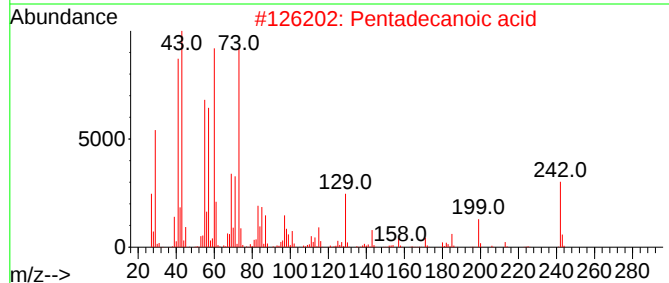
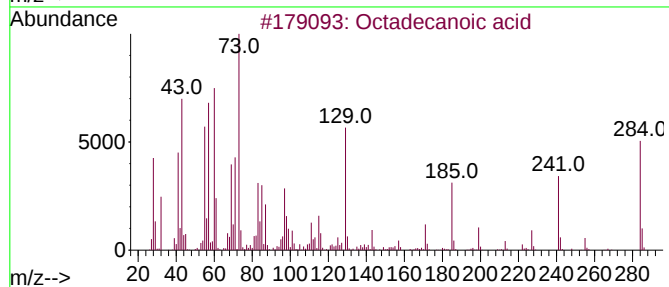
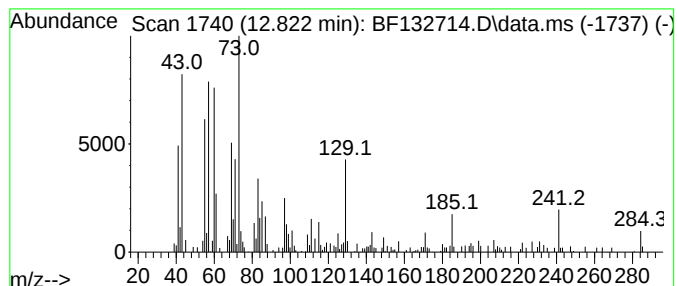
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.822	2.07 ng	135657	Phenanthrene-d10	11.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68



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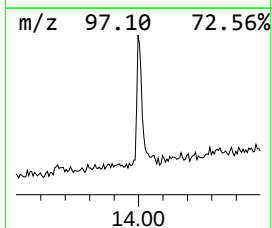
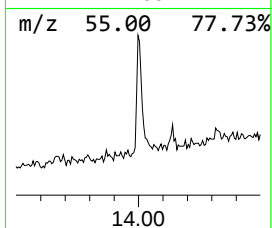
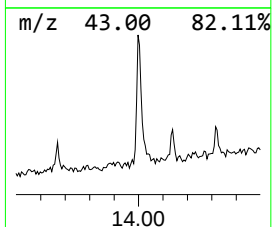
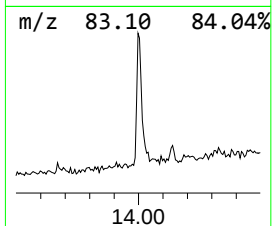
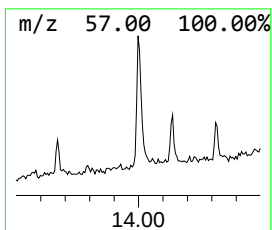
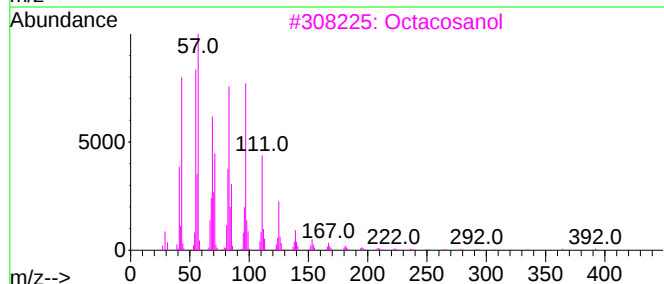
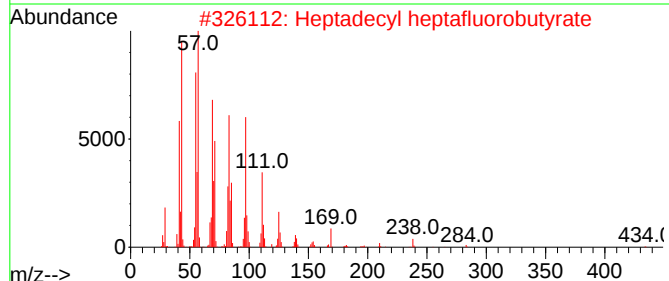
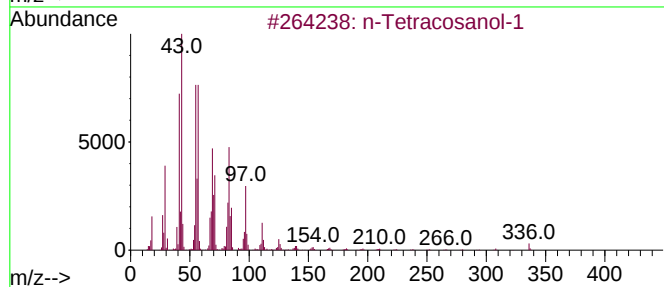
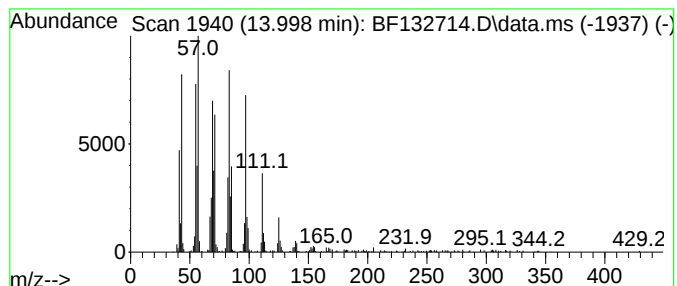
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TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	7.35 ng	409802	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Octacosanol	410	C28H58O	000557-61-9	91
4			1-Heptacosanol	396	C27H56O	002004-39-9	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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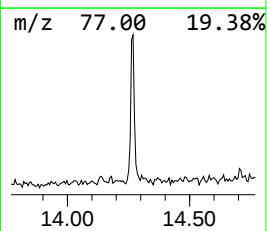
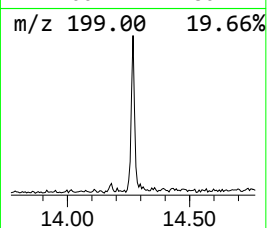
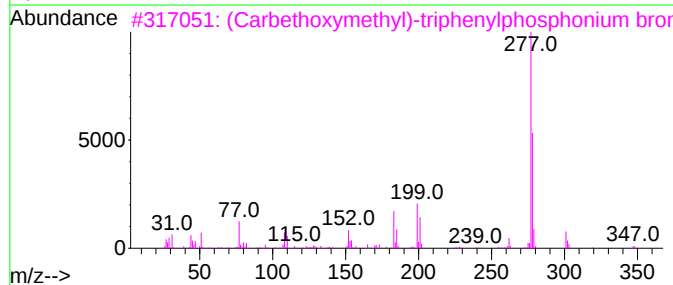
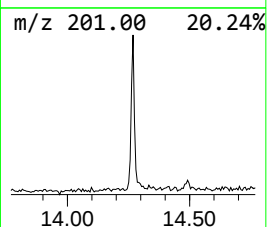
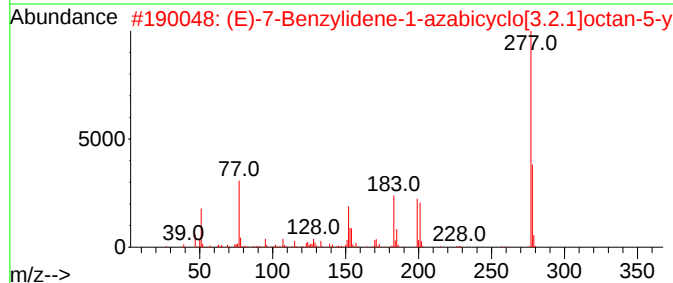
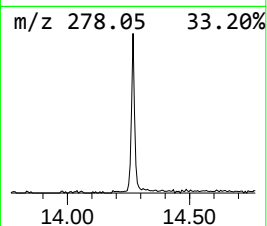
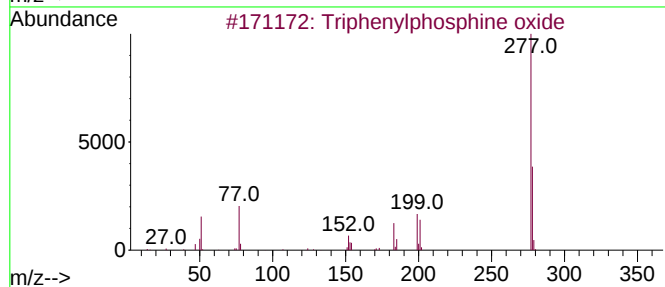
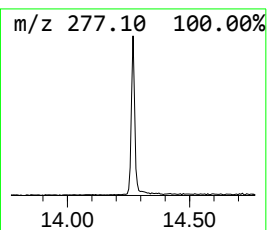
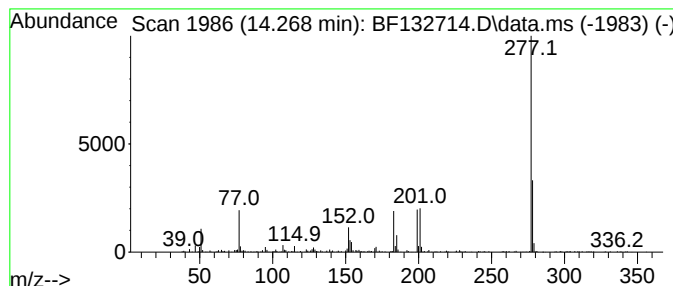
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.269	3.92 ng	218710	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	52
3			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	45
4			5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	38
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030923\
Data File : BF132714.D
Acq On : 09 Mar 2023 12:57
Operator : CG\JU
Sample : 01829-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SS-02-20230306

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-...	5.204	29.2	ng	1588790	1	6.981	1086730	20.0
Benzophenone	10.739	8.6	ng	651551	3	10.028	1523890	20.0
n-Hexadecanoic ...	12.033	5.1	ng	331981	4	11.522	1308870	20.0
Octadecanoic acid	12.822	2.1	ng	135657	4	11.522	1308870	20.0
n-Tetracosanol-1	13.998	7.3	ng	409802	5	14.180	1115250	20.0
Triphenylphosph...	14.269	3.9	ng	218710	5	14.180	1115250	20.0