

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
 Data File : BF133303.D
 Acq On : 08 May 2023 19:40
 Operator : CG\JU
 Sample : 02660-02
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WATER-SAMPLE-API-3-6

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-BF042123.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133303.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.051	160	164	176	rBV	77042	172365	2.95%	0.529%
2	4.898	474	478	486	rVB	602246	650797	11.15%	1.998%
3	5.328	547	551	558	rBV	2664684	2394837	41.05%	7.354%
4	5.728	615	619	626	rBV	115669	116559	2.00%	0.358%
5	6.357	723	726	734	rBV	1761230	1453381	24.91%	4.463%
6	6.722	784	788	791	rBV	1387306	1165417	19.97%	3.579%
7	6.781	795	798	803	rVB2	78849	64423	1.10%	0.198%
8	7.286	878	884	887	rBV	3619833	3636422	62.33%	11.167%
9	8.004	1002	1006	1009	rVB	2140410	1527941	26.19%	4.692%
10	8.375	1064	1069	1072	rBV4	31990	60754	1.04%	0.187%
11	8.428	1076	1078	1084	rVV5	48979	71690	1.23%	0.220%
12	9.080	1185	1189	1192	rVB	5960233	5834554	100.00%	17.917%
13	9.616	1277	1280	1282	rBV	105491	116697	2.00%	0.358%
14	9.657	1285	1287	1289	rVB	99808	71224	1.22%	0.219%
15	9.757	1300	1304	1307	rBV	2086211	1684404	28.87%	5.172%
16	9.822	1312	1315	1317	rBV3	62647	63785	1.09%	0.196%
17	10.022	1347	1349	1351	rBV2	101288	82833	1.42%	0.254%
18	10.257	1386	1389	1395	rBV3	218211	242099	4.15%	0.743%
19	10.310	1395	1398	1399	rBV3	117795	114254	1.96%	0.351%
20	10.469	1423	1425	1429	rBV	286433	313034	5.37%	0.961%
21	10.545	1434	1438	1441	rVV	3101902	3158198	54.13%	9.698%
22	11.080	1527	1529	1531	rBV	127696	116692	2.00%	0.358%
23	11.239	1553	1556	1559	rVB	1867291	1462466	25.07%	4.491%
24	11.786	1645	1649	1652	rBV	653992	632493	10.84%	1.942%
25	12.563	1779	1781	1786	rVB	364201	351538	6.03%	1.080%
26	12.827	1822	1826	1829	rBV	4704788	4373527	74.96%	13.430%
27	13.739	1978	1981	1993	rVB	259097	380759	6.53%	1.169%
28	13.874	2000	2004	2007	rBV	1071878	940975	16.13%	2.890%
29	13.980	2019	2022	2026	rVB	299146	270577	4.64%	0.831%
30	15.292	2241	2245	2250	rVB	953590	1039994	17.82%	3.194%

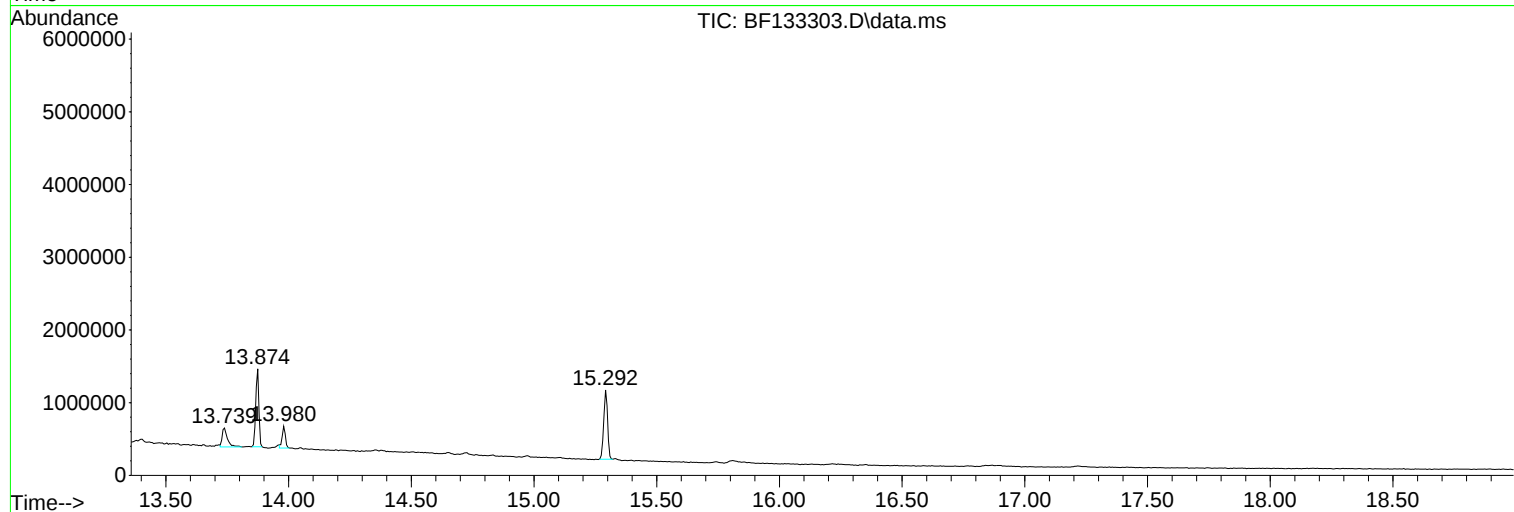
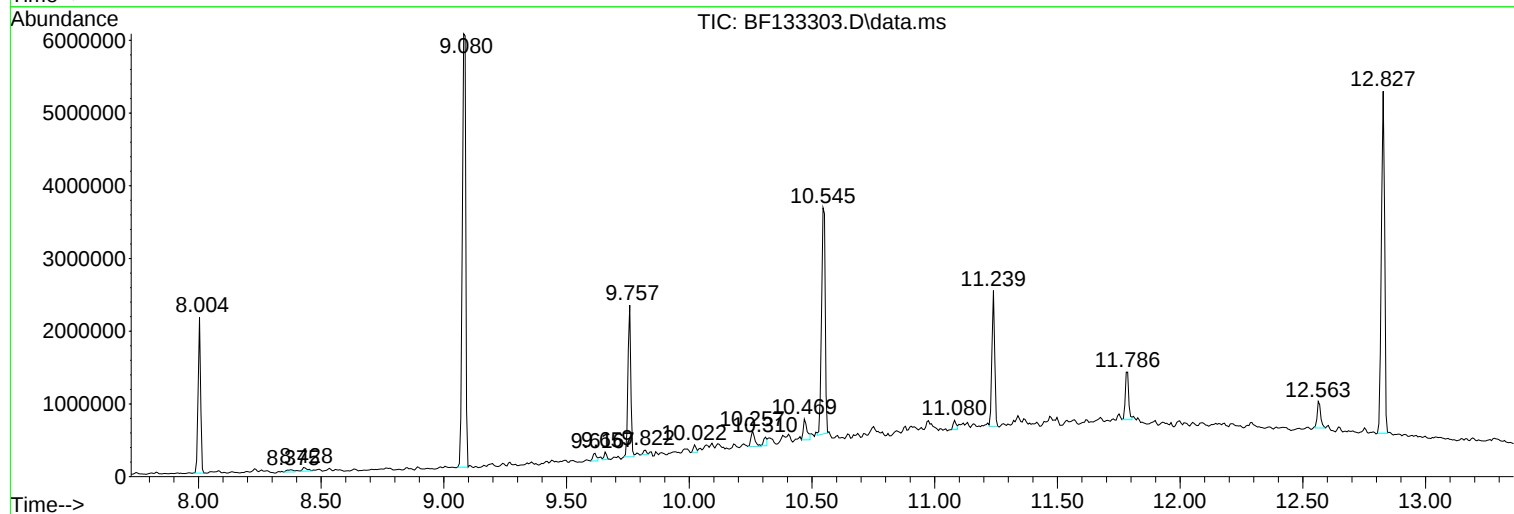
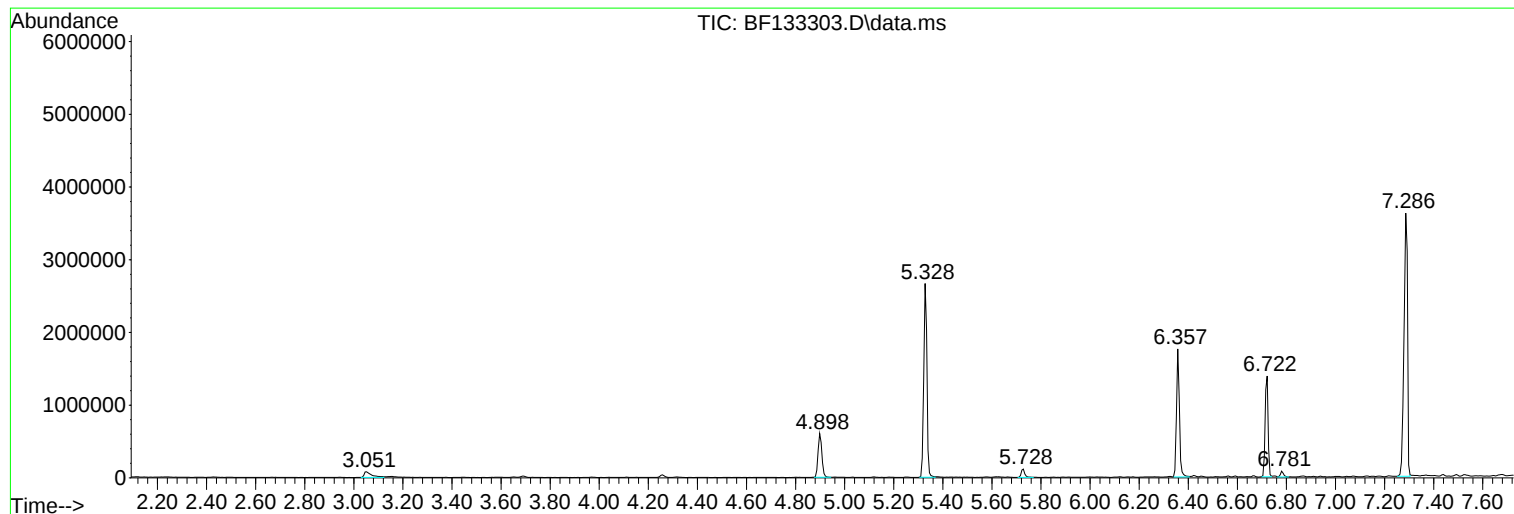
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ALS Vial : 18 Sample Multiplier: 1

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ClientSampleId :
WATER-SAMPLE-API-3-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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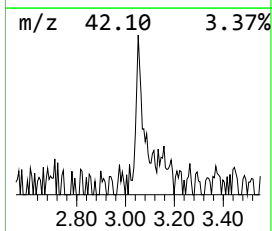
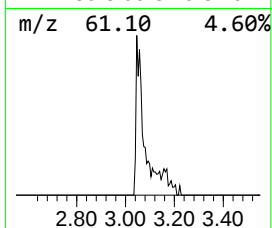
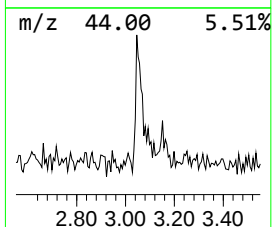
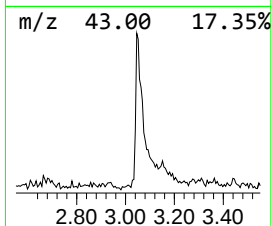
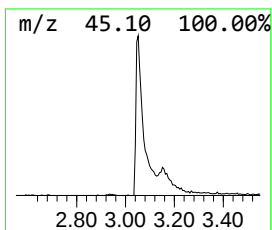
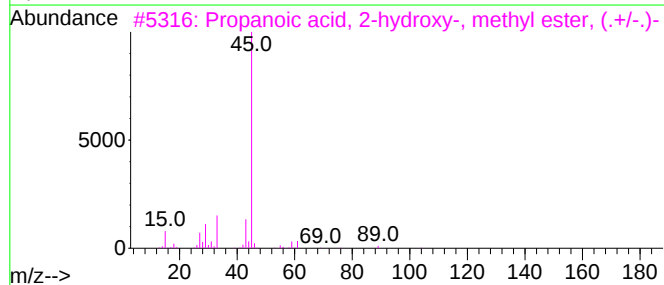
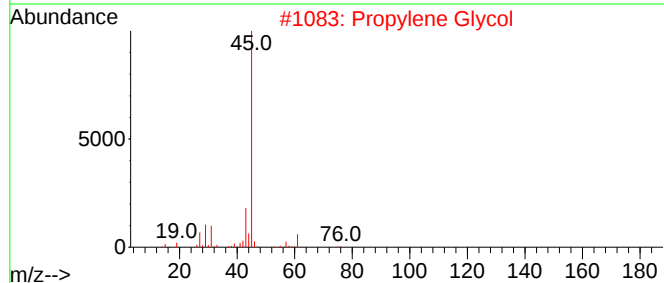
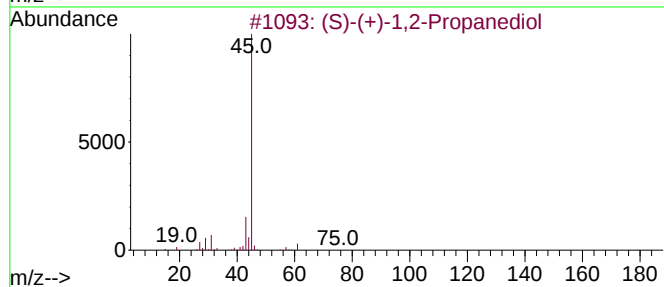
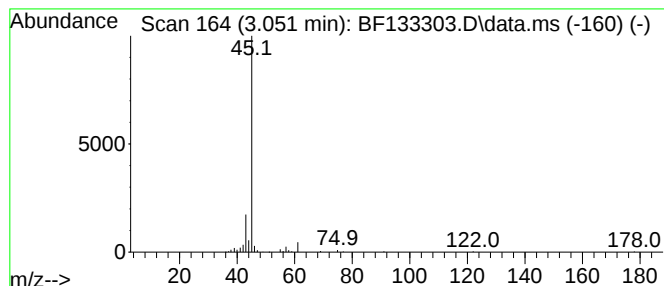
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.051	2.96 ng	172365	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	56
2	Propylene Glycol			76	C3H8O2	000057-55-6	43
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	40
4	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	40
5	2-Hexanol			102	C6H14O	000626-93-7	9



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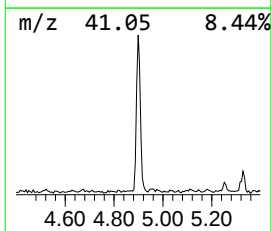
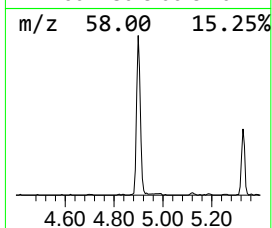
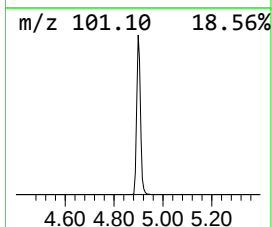
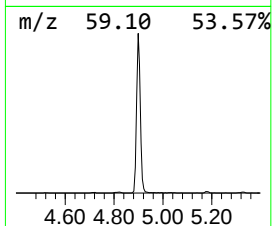
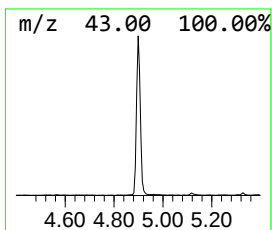
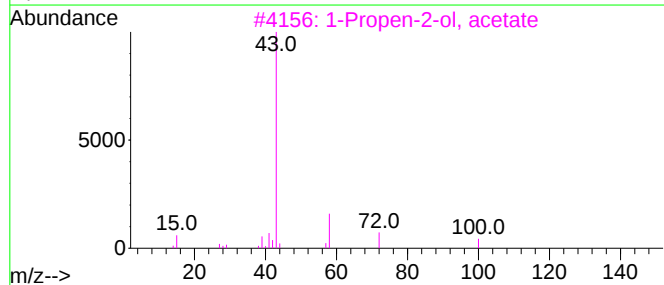
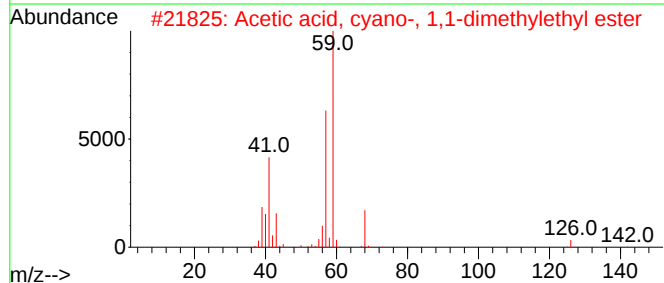
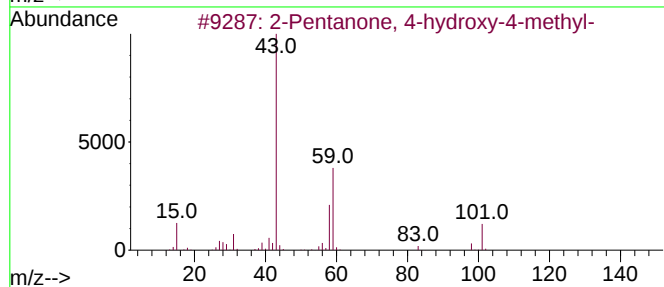
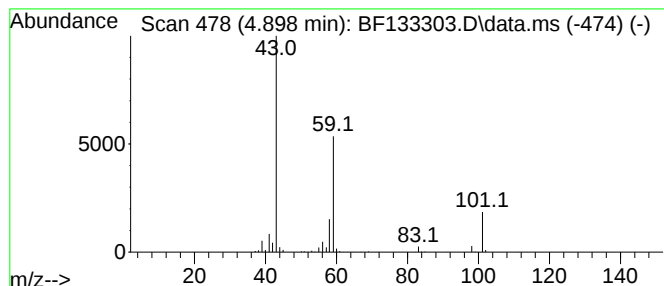
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.898	11.17 ng	650797	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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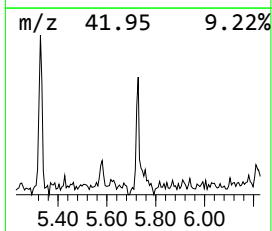
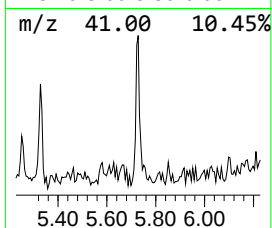
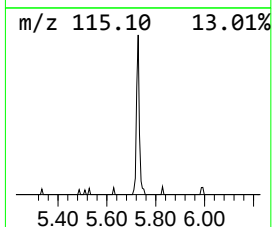
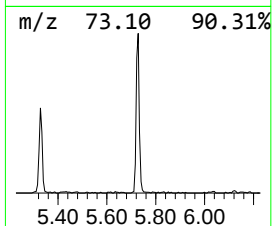
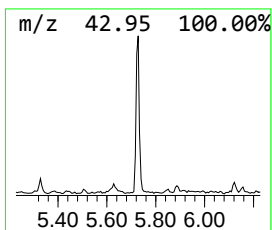
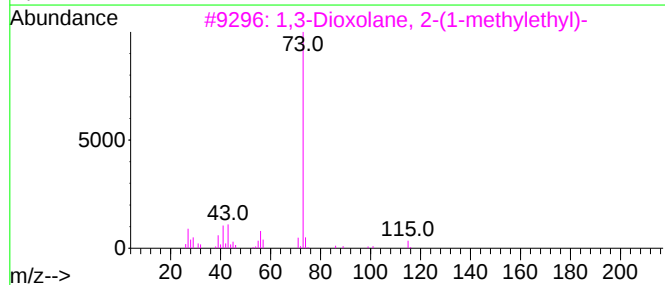
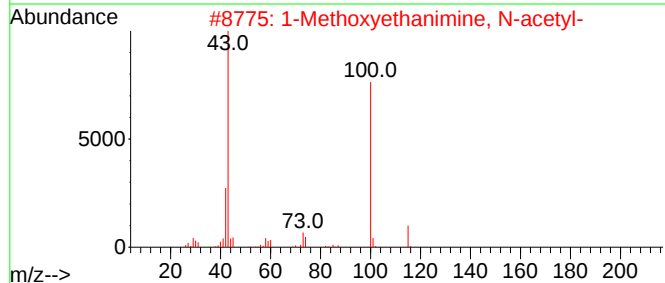
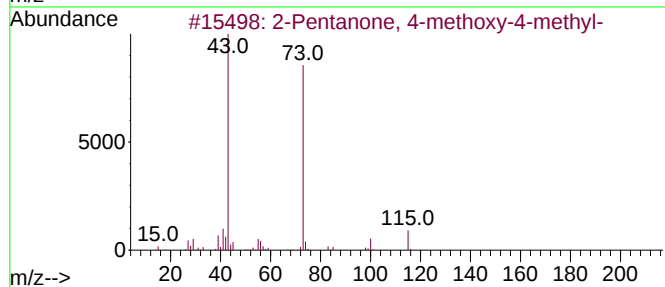
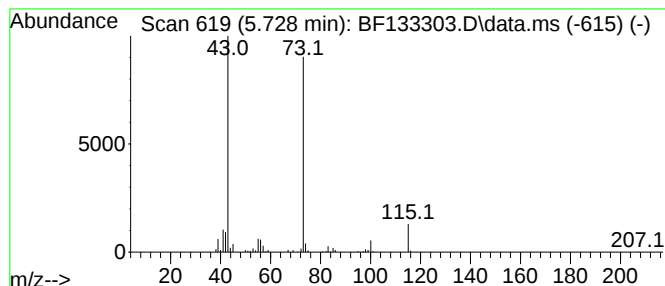
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.728	2.00 ng	116559	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	22
4			N-Formylmorpholine	115	C5H9NO2	004394-85-8	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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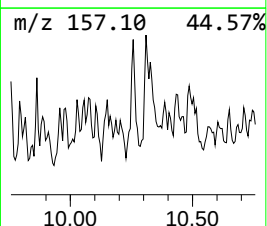
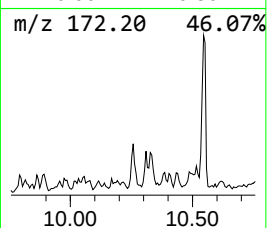
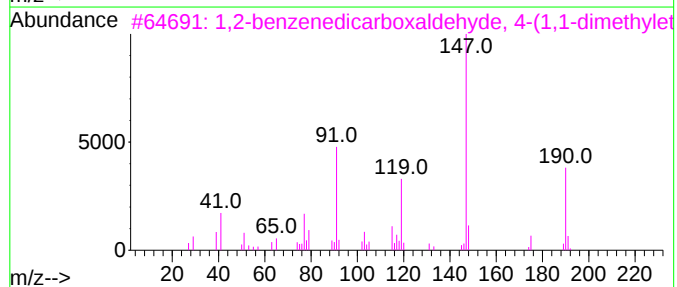
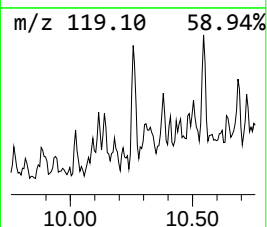
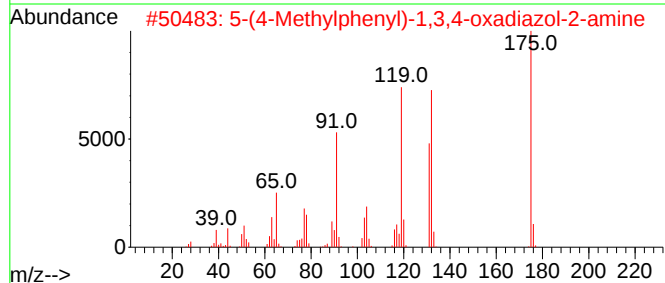
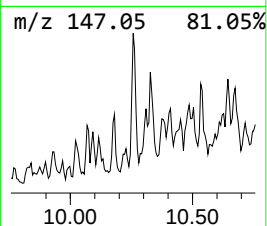
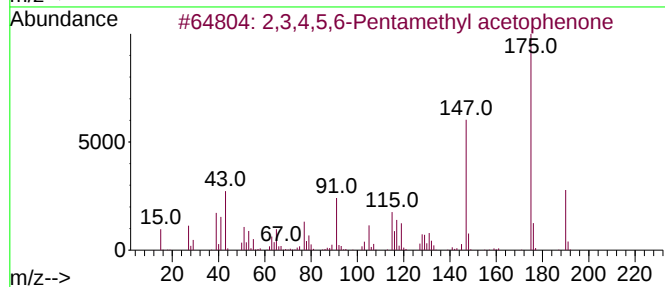
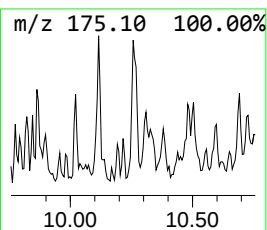
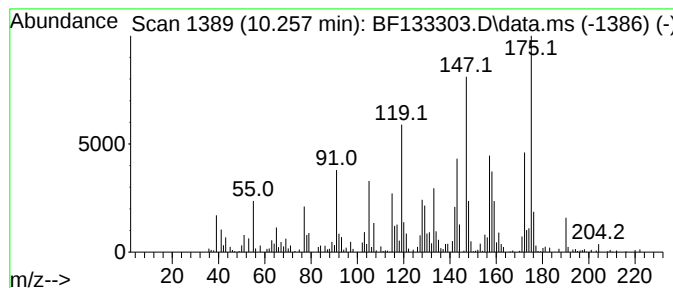
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Peak Number 4 unknown10.257 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.257	2.87 ng	242099	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4,5,6-Pentamethyl acetophenone	190	C13H18O	1000342-53-1	27		
2	5-(4-Methylphenyl)-1,3,4-oxadiaz...	175	C9H9N3O	033621-60-2	18		
3	1,2-benzenedicarboxaldehyde, 4-(...	190	C12H14O2	1010400-21-4	15		
4	2-Propenal, 3-[4-(dimethylamino)...]	175	C11H13NO	006203-18-5	15		
5	Pyrido[3,2-d]pyrimidin-4-ol	147	C7H5N3O	037538-67-3	14		



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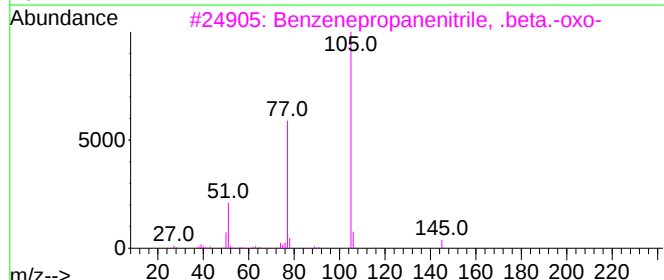
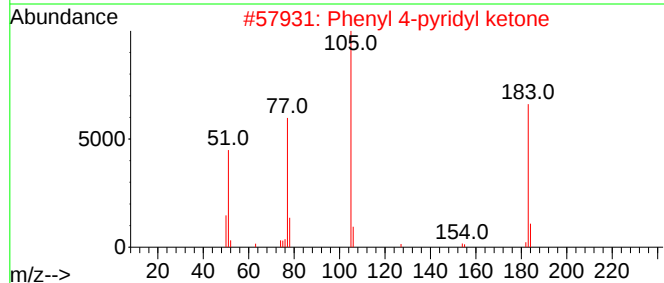
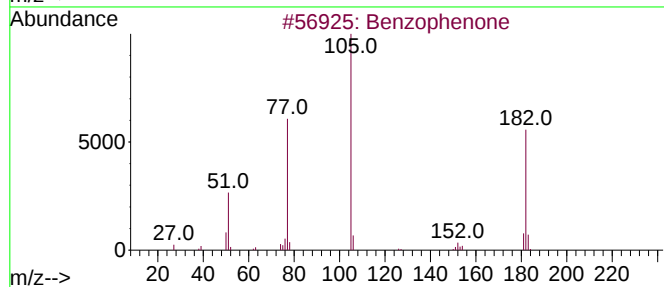
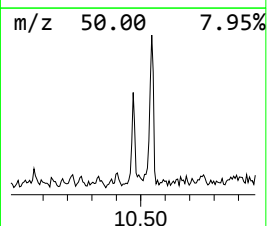
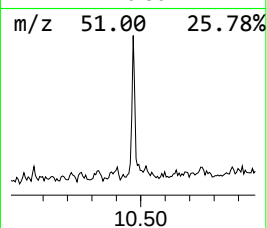
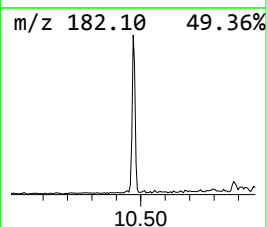
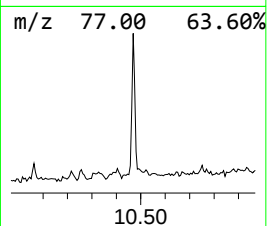
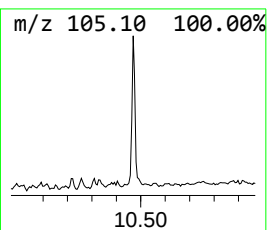
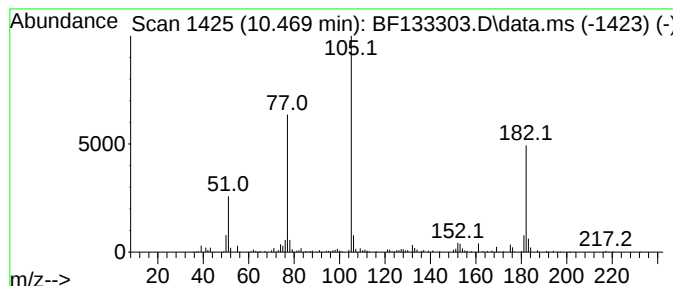
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Peak Number 5 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.469	3.72 ng	313034	Acenaphthene-d10	9.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
3			Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
4			cis-Cyclopentanecarboxylic acid,...	250	C13H14O3S	099397-53-2	43
5			N-Benzoylimidazole	172	C10H8N2O	010364-94-0	43



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ClientSampleId :
WATER-SAMPLE-API-3-6

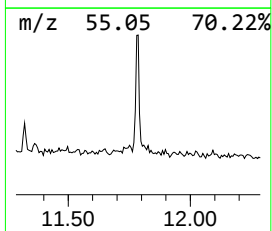
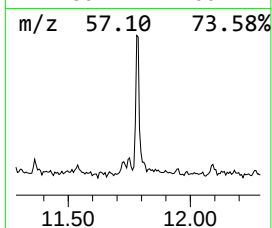
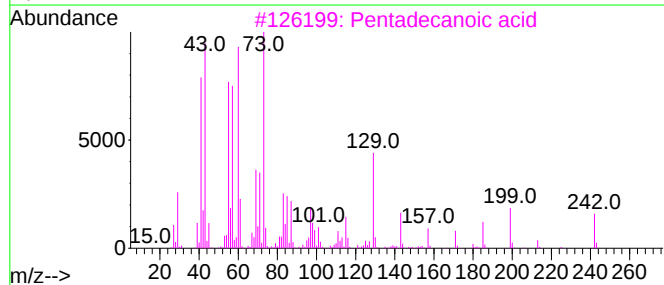
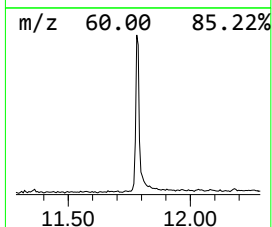
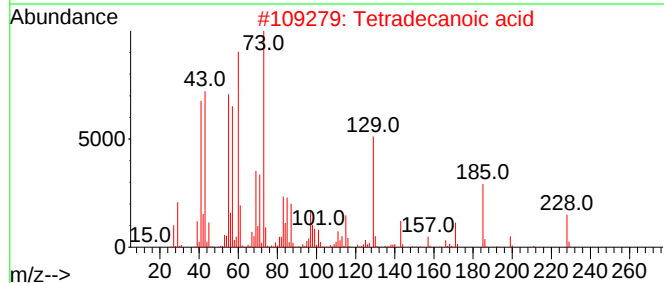
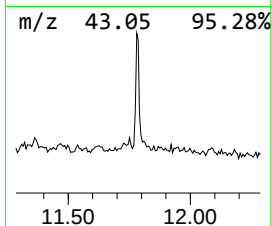
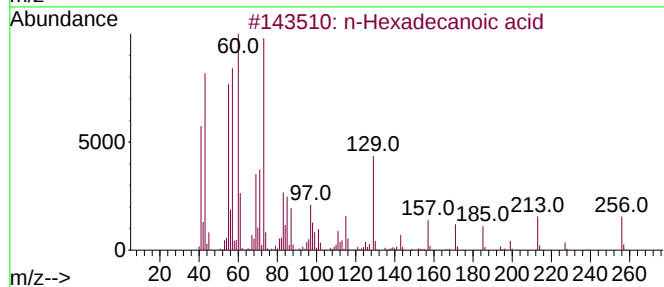
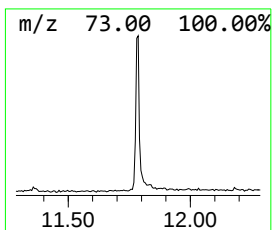
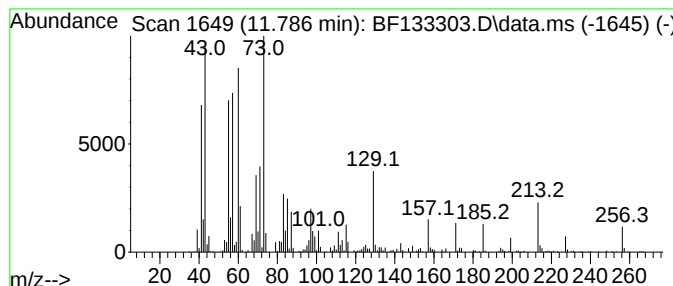
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	8.65 ng	632493	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Nonanoic acid	158	C9H18O2	000112-05-0	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133303.D
Acq On : 08 May 2023 19:40
Operator : CG\JU
Sample : 02660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-6

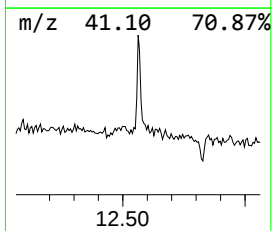
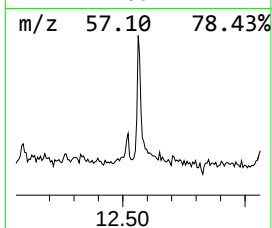
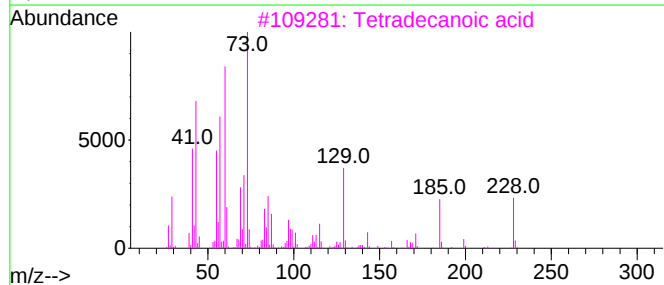
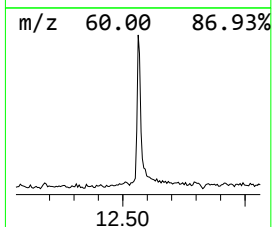
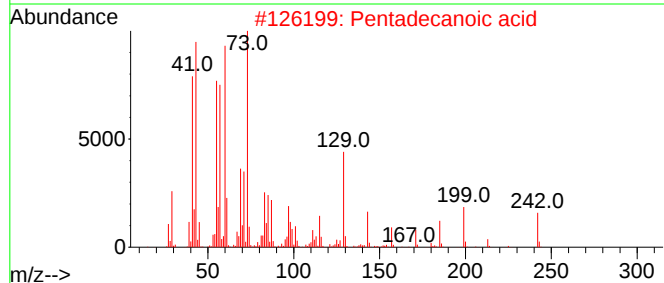
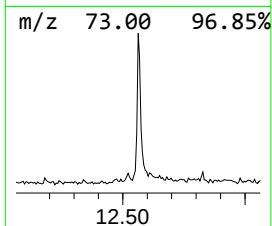
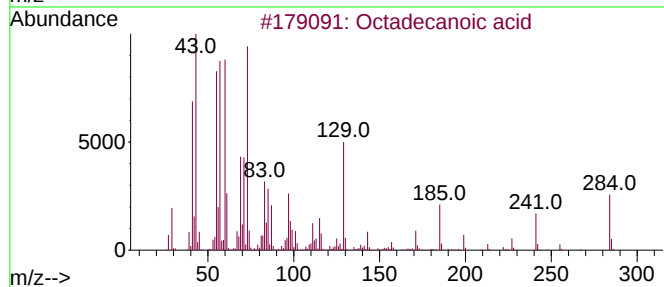
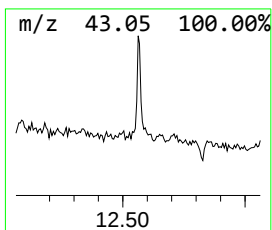
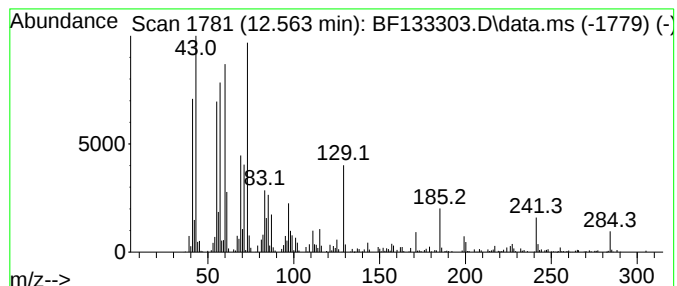
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	7.47 ng	351538	Chrysene-d12	13.874

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133303.D
Acq On : 08 May 2023 19:40
Operator : CG\JU
Sample : 02660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-6

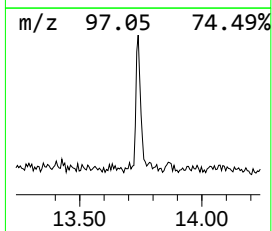
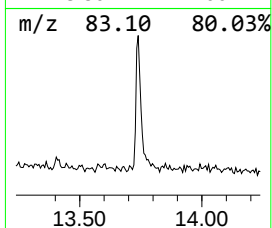
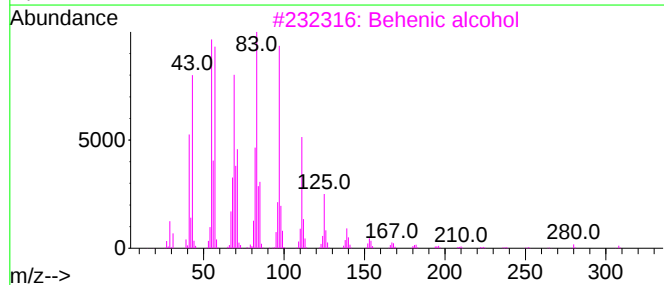
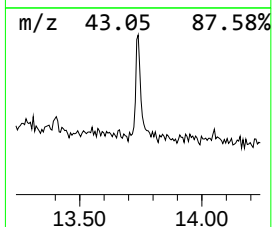
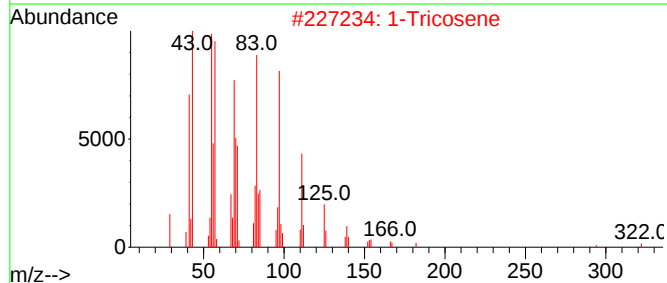
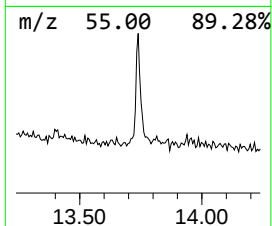
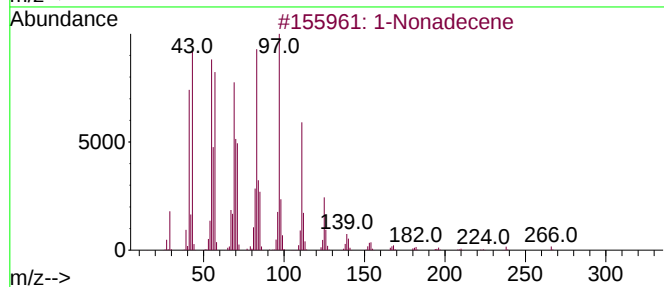
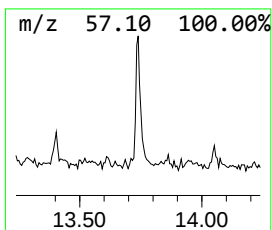
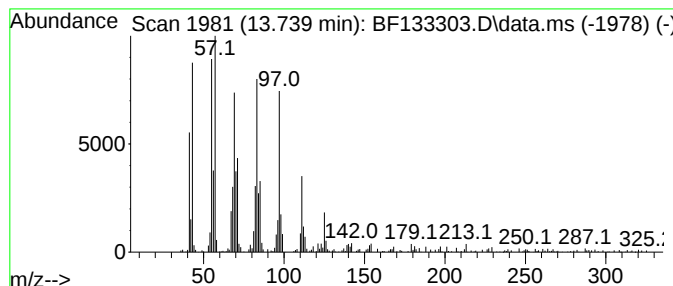
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.739	8.09 ng	380759	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonadecene	266	C19H38	018435-45-5	97
2			1-Tricosene	322	C23H46	018835-32-0	94
3			Behenic alcohol	326	C22H46O	000661-19-8	94
4			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	94
5			1-Heneicosanol	312	C21H44O	015594-90-8	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133303.D
Acq On : 08 May 2023 19:40
Operator : CG\JU
Sample : 02660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-6

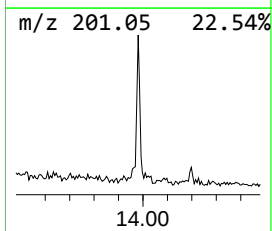
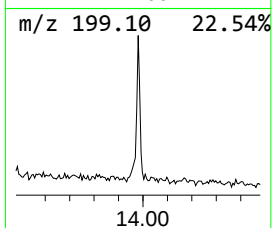
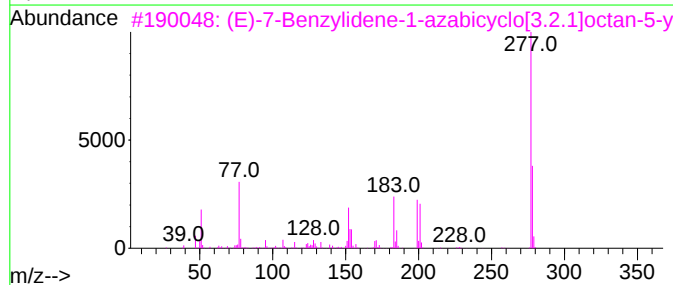
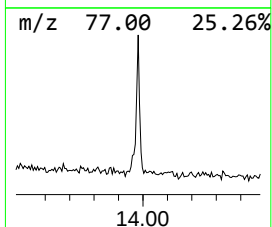
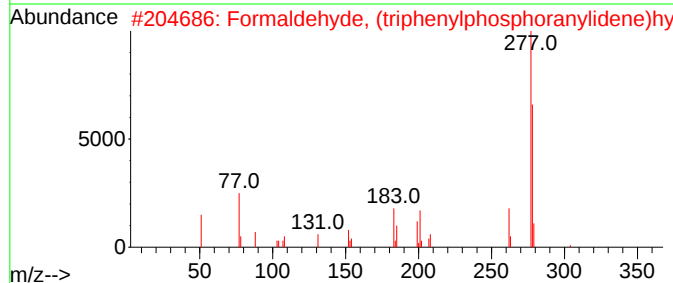
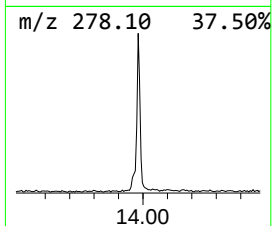
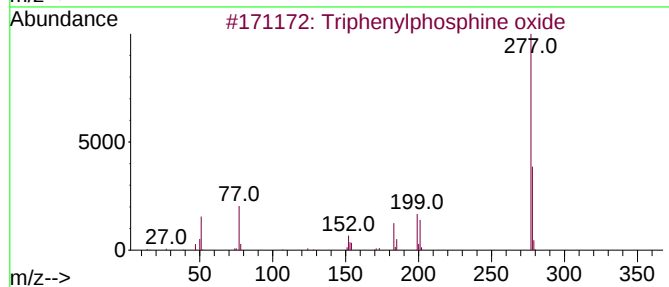
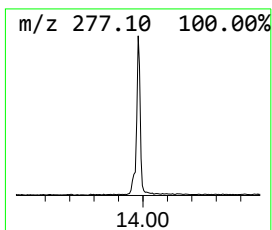
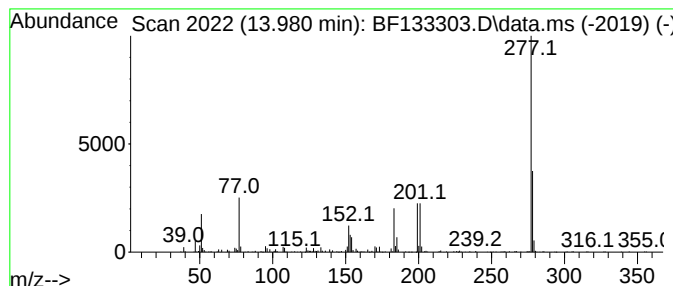
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	5.75 ng	270577	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	95
2			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	59
3			(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19N03S	1000483-83-4	47
4			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050823\
Data File : BF133303.D
Acq On : 08 May 2023 19:40
Operator : CG\JU
Sample : 02660-02
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WATER-SAMPLE-API-3-6

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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					#	RT	Resp	Conc
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2-Pentanone, 4-...	4.898	11.2	ng	650797	1	6.722	1165420	20.0
2-Pentanone, 4-...	5.728	2.0	ng	116559	1	6.722	1165420	20.0
unknown10.257	10.257	2.9	ng	242099	3	9.757	1684400	20.0
Benzophenone	10.469	3.7	ng	313034	3	9.757	1684400	20.0
n-Hexadecanoic ...	11.786	8.7	ng	632493	4	11.239	1462470	20.0
Octadecanoic acid	12.563	7.5	ng	351538	5	13.874	940975	20.0
1-Nonadecene	13.739	8.1	ng	380759	5	13.874	940975	20.0
Triphenylphosph...	13.980	5.8	ng	270577	5	13.874	940975	20.0