

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
 Data File : BF131917.D
 Acq On : 05 Jan 2023 16:17
 Operator : CG\JU
 Sample : 01029-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-205

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-BF122422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131917.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	4	8	14	rVB	48648	58632	2.22%	0.301%
2	5.010	491	497	508	rVB	634067	893490	33.86%	4.587%
3	5.416	561	566	569	rBV	2172874	2092043	79.29%	10.740%
4	6.439	735	740	743	rBV	2025180	2160432	81.88%	11.091%
5	6.798	798	801	805	rBV	476937	413387	15.67%	2.122%
6	7.375	893	899	902	rBV	1459142	1435564	54.41%	7.369%
7	8.092	1016	1021	1024	rBV	569086	518854	19.66%	2.664%
8	9.175	1199	1205	1208	rBV	2924892	2638511	100.00%	13.545%
9	9.480	1253	1257	1260	rBV	84154	70305	2.66%	0.361%
10	9.851	1315	1320	1324	rVB	749510	634732	24.06%	3.258%
11	9.992	1339	1344	1347	rBV	1433032	1326109	50.26%	6.808%
12	10.298	1394	1396	1404	rVB	46616	43824	1.66%	0.225%
13	10.363	1404	1407	1411	rVB	144955	112516	4.26%	0.578%
14	10.575	1438	1443	1446	rBV	708880	567288	21.50%	2.912%
15	10.651	1450	1456	1459	rBV	1999115	1811948	68.67%	9.302%
16	10.727	1466	1469	1478	rVB	43609	50682	1.92%	0.260%
17	11.345	1570	1574	1577	rBV	855237	670182	25.40%	3.440%
18	11.880	1658	1665	1675	rBV	157477	194321	7.36%	0.998%
19	12.063	1693	1696	1703	rVB4	19746	30723	1.16%	0.158%
20	12.127	1703	1707	1710	rBV	61740	52923	2.01%	0.272%
21	12.945	1841	1846	1849	rBV	2847276	2450700	92.88%	12.581%
22	13.839	1993	1998	2012	rBV	209237	298585	11.32%	1.533%
23	13.998	2016	2025	2029	rBV	441869	406835	15.42%	2.088%
24	14.163	2046	2053	2058	rBV4	18050	31326	1.19%	0.161%
25	14.851	2166	2170	2176	rVB	37083	42258	1.60%	0.217%
26	15.474	2271	2276	2284	rBV	298642	384206	14.56%	1.972%
27	16.004	2360	2366	2378	rBV10	18182	61089	2.32%	0.314%
28	17.533	2618	2626	2628	rBV8	11233	28366	1.08%	0.146%

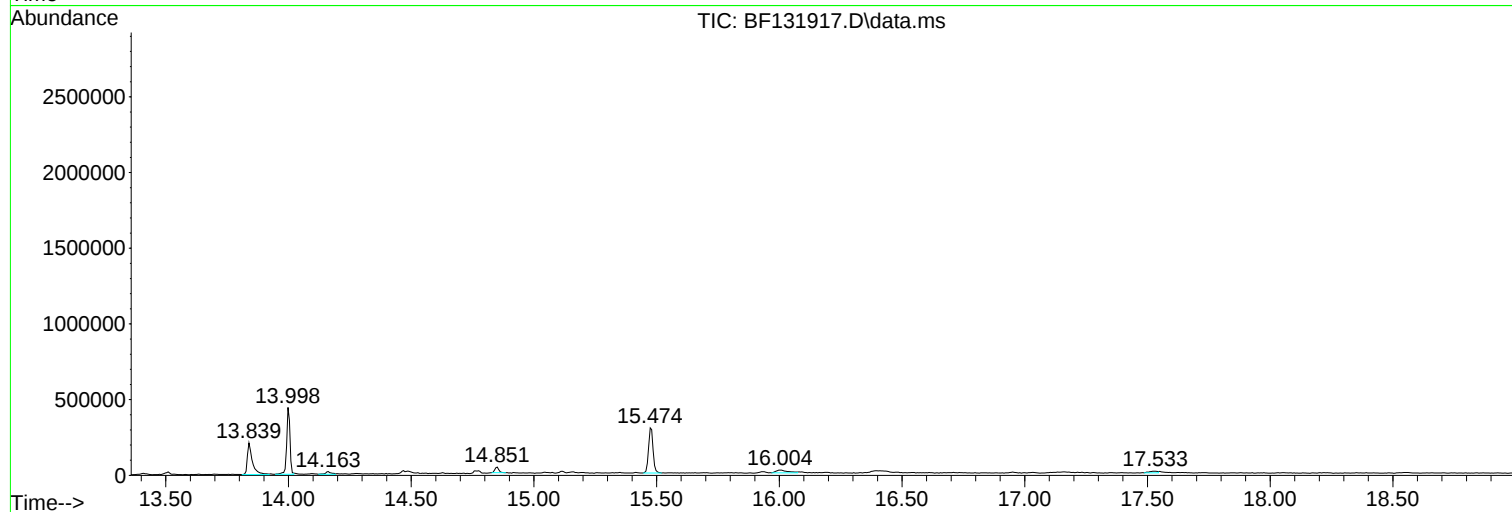
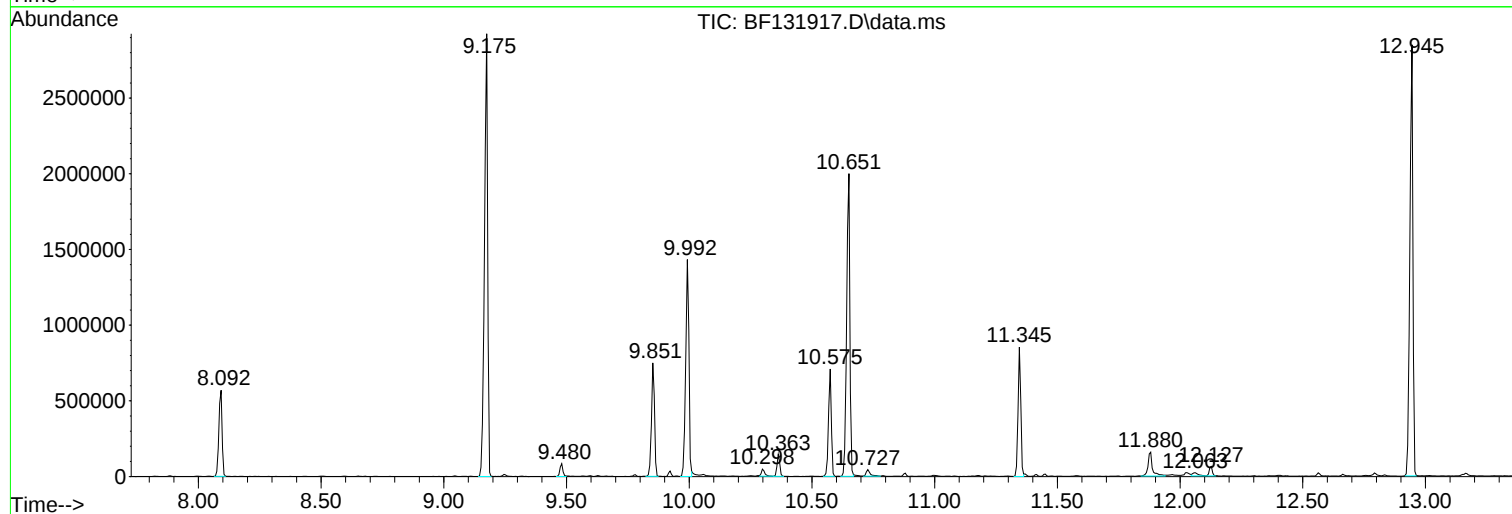
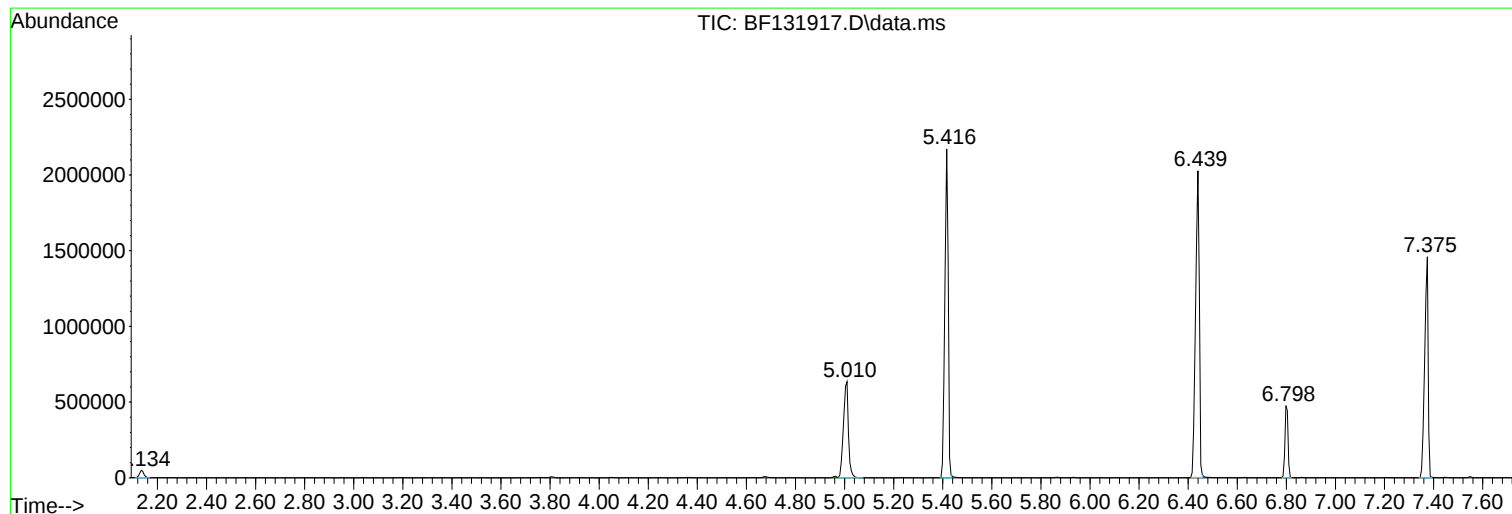
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-205

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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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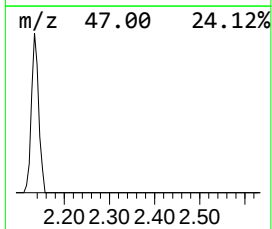
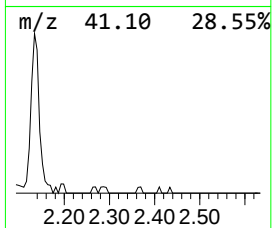
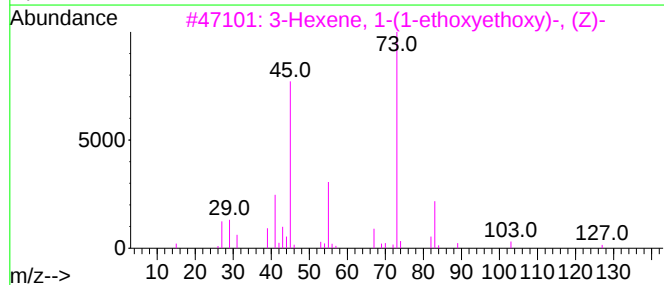
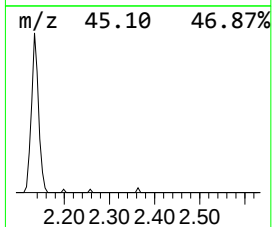
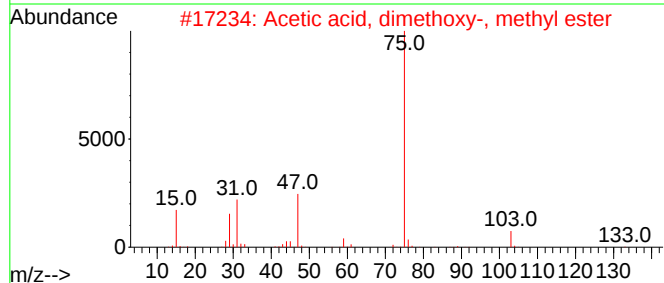
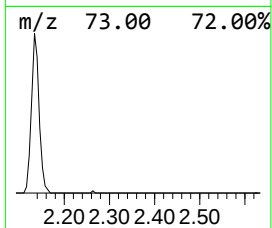
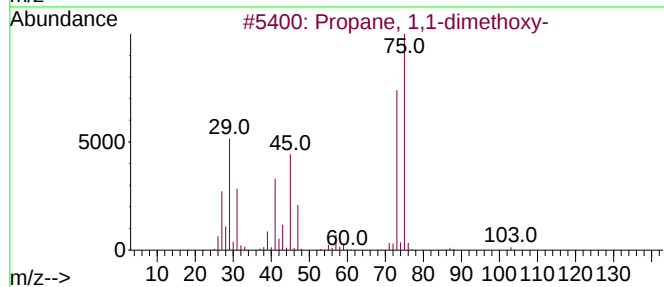
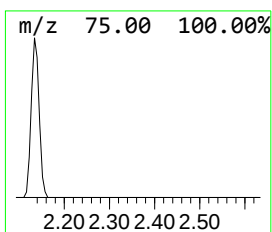
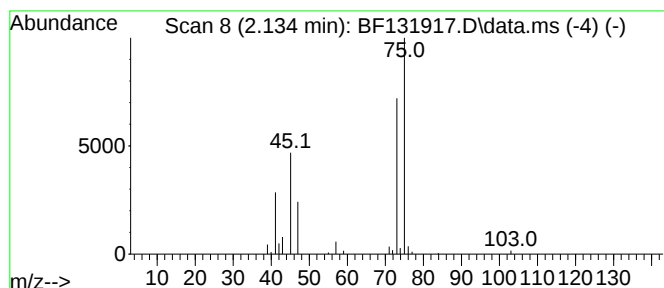
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.84 ng	58632	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Acetic acid, dimethoxy-, methyl ...	134	C5H10O4	000089-91-8	9
3			3-Hexene, 1-(1-ethoxyethoxy)-, (Z)-	172	C10H20O2	028069-74-1	9
4			Ethane, 1,1,2-trimethoxy-	120	C5H12O3	024332-20-5	9
5			Propanoic acid, 2,3-dihydroxy-	106	C3H6O4	000473-81-4	9



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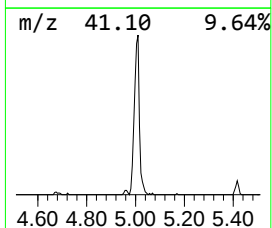
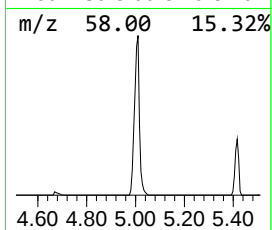
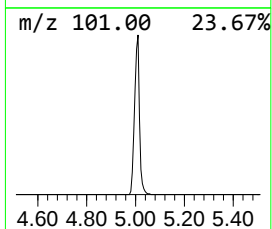
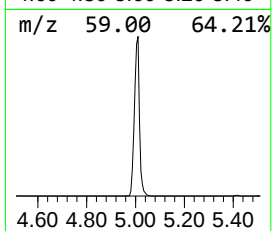
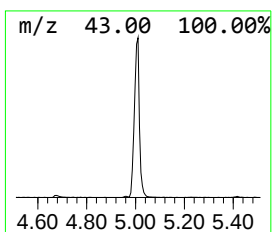
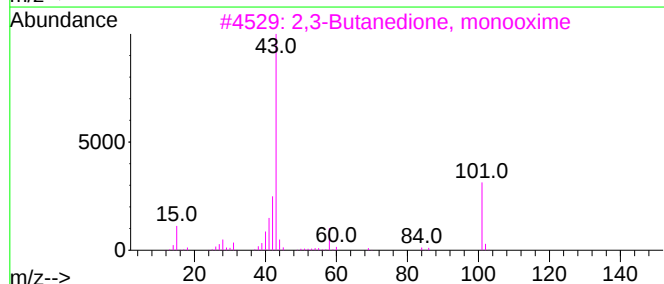
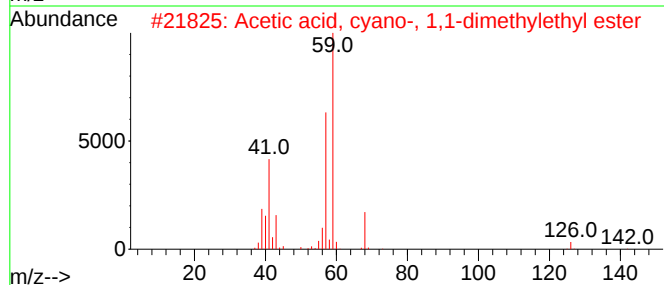
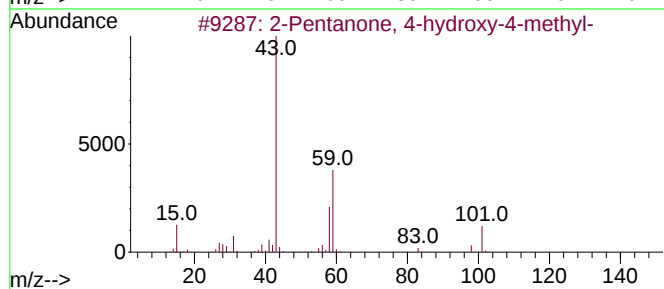
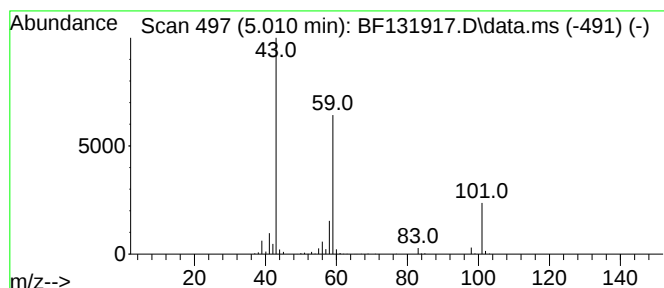
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	43.23 ng	893490	1,4-Dichlorobenzene-d4	6.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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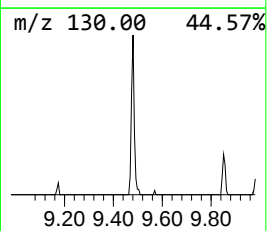
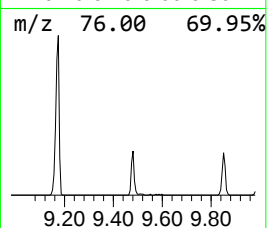
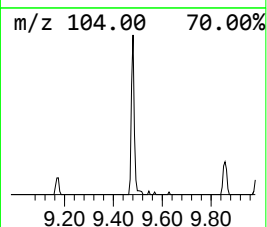
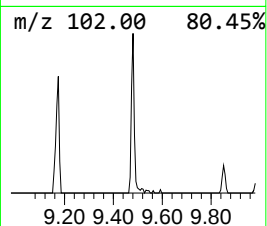
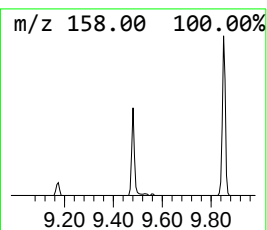
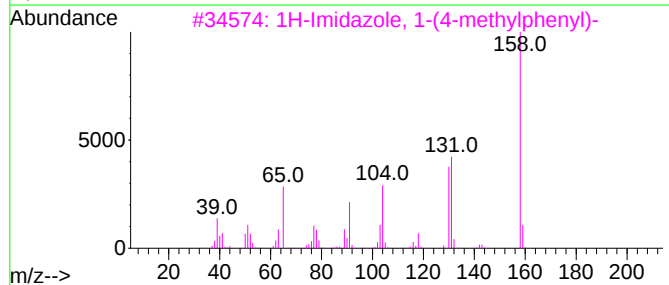
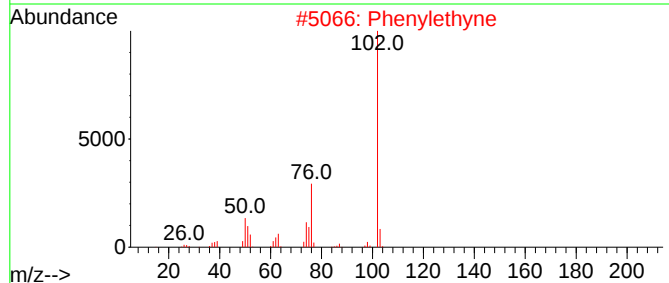
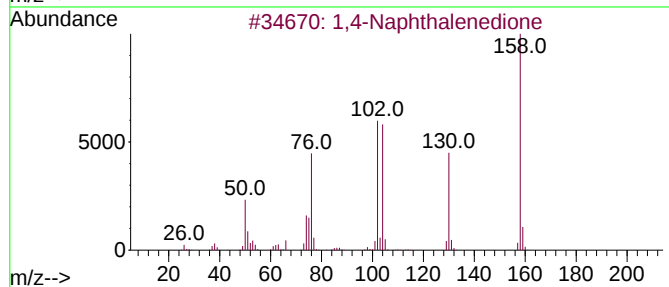
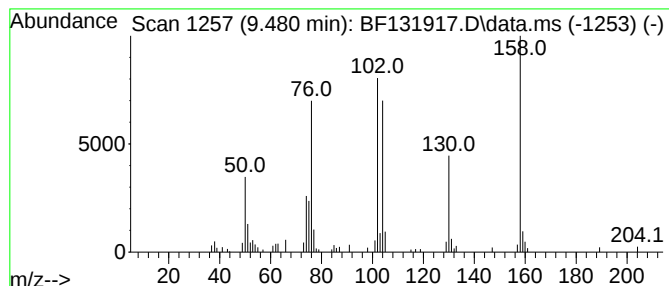
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1,4-Naphthalenedione Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.480	2.22 ng	70305	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Naphthalenedione	158	C10H6O2	000130-15-4	97
2			Phenylethyne	102	C8H6	000536-74-3	46
3			1H-Imidazole, 1-(4-methylphenyl)-	158	C10H10N2	1000351-29-5	30
4			2,3-Naphthalenediamine	158	C10H10N2	000771-97-1	25
5			1,4-Naphthalenediamine	158	C10H10N2	002243-61-0	22



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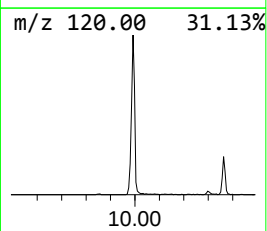
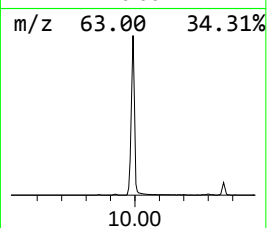
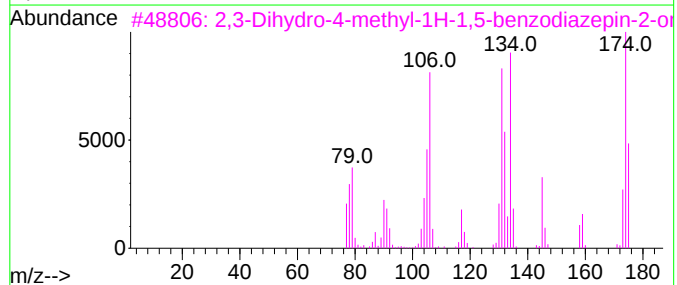
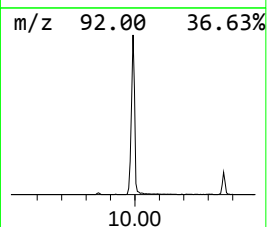
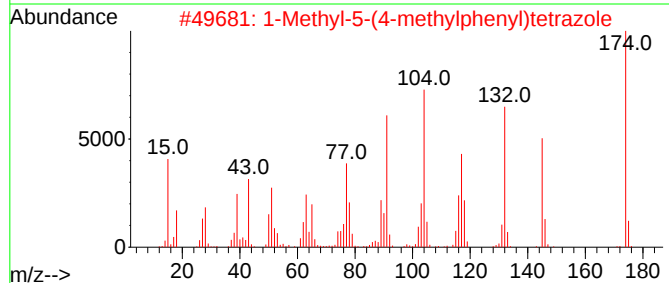
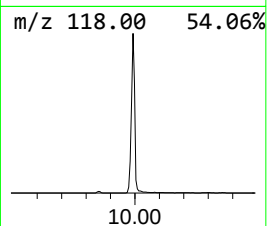
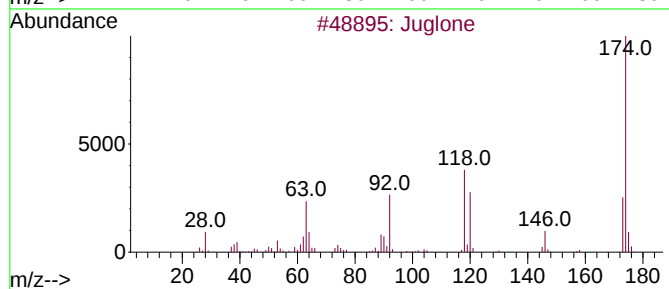
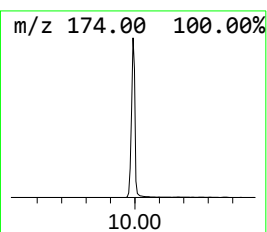
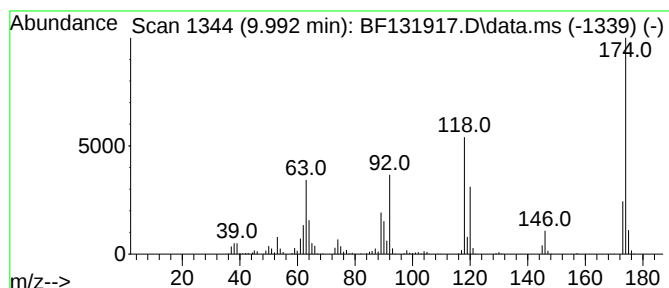
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Peak Number 4 Juglone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.992	41.78 ng	1326110	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Juglone	174	C10H6O3	000481-39-0	97
2			1-Methyl-5-(4-methylphenyl)tetra...	174	C9H10N4	068826-33-5	52
3			2,3-Dihydro-4-methyl-1H-1,5-benz...	174	C10H10N2O	006276-48-8	46
4			3-(3-Methoxyphenyl)-1H-pyrazole	174	C10H10N2O	1000410-63-5	46
5			Benzene, 2,4-diisocyanato-1-methyl-	174	C9H6N2O2	000584-84-9	35



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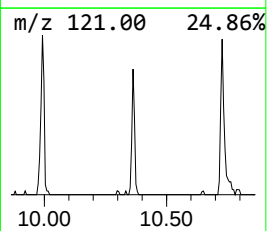
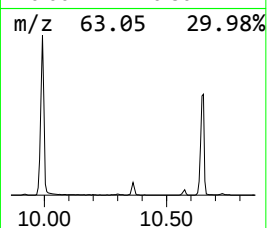
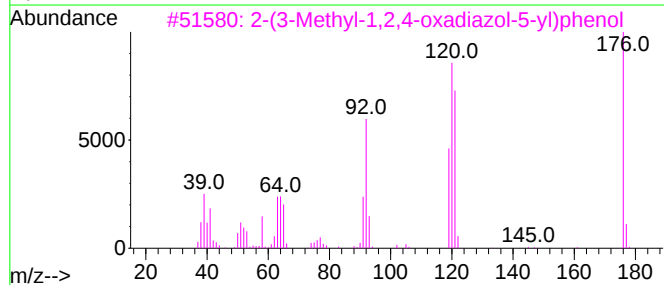
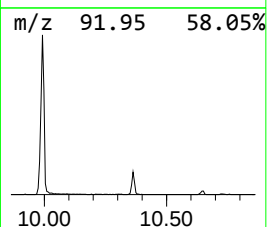
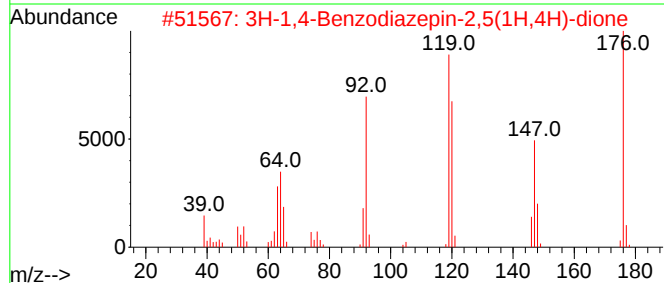
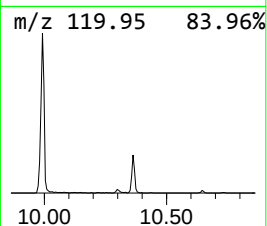
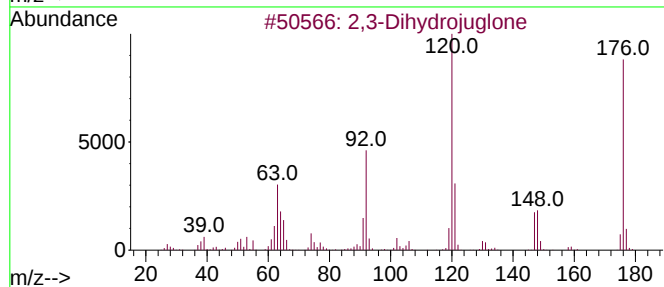
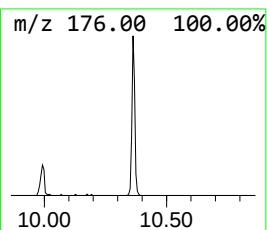
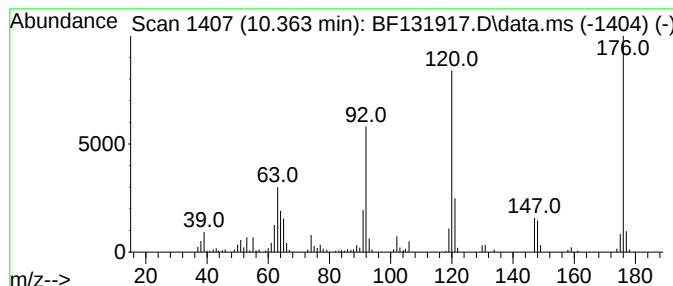
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Peak Number 5 2,3-Dihydrojuglone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.363	3.55 ng	112516	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,3-Dihydrojuglone	176	C10H8O3	006312-53-4	96
2			3H-1,4-Benzodiazepin-2,5(1H,4H)-...	176	C9H8N2O2	005118-94-5	80
3			2-(3-Methyl-1,2,4-oxadiazol-5-yl)...	176	C9H8N2O2	1000411-33-9	64
4			7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	43
5			2-Hydroxy-3-cyanopyridine	120	C6H4N2O	020577-27-9	38



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TP-205

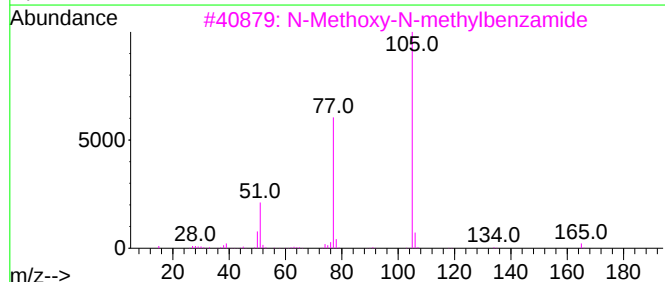
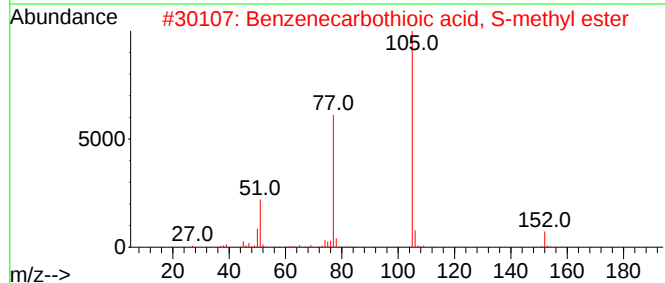
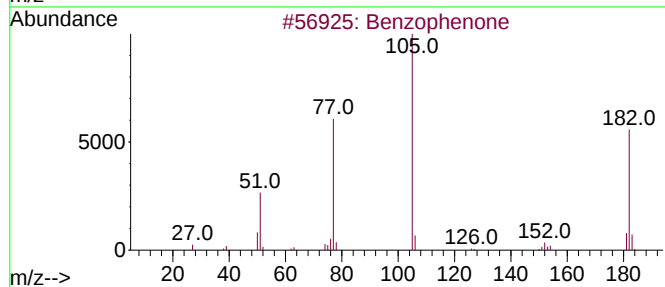
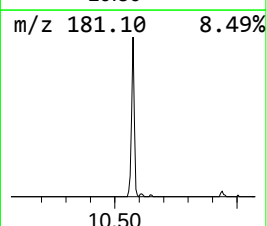
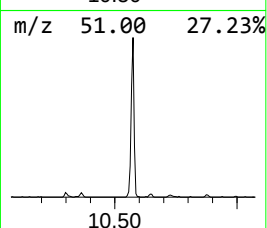
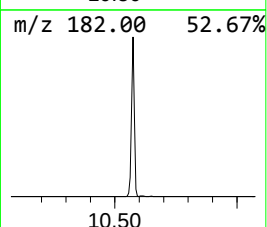
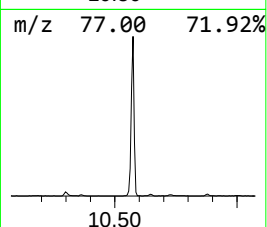
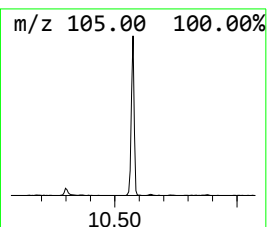
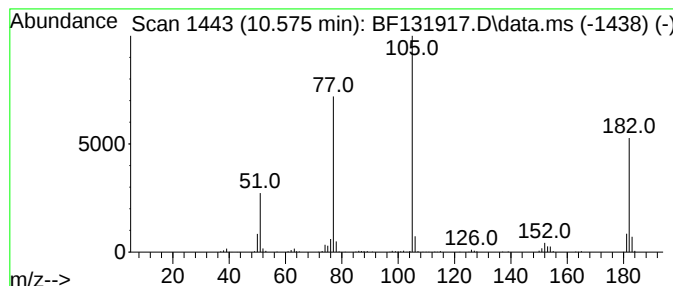
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	17.87 ng	567288	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
4			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47
5			Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131917.D
Acq On : 05 Jan 2023 16:17
Operator : CG\JU
Sample : 01029-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-205

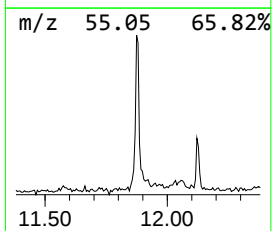
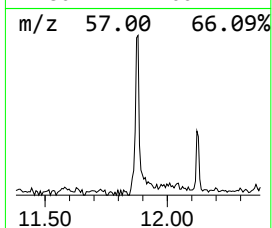
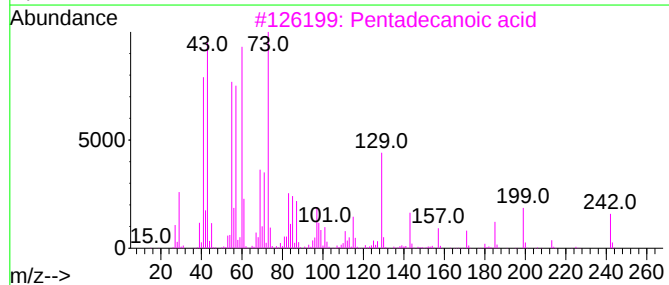
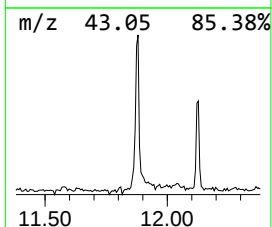
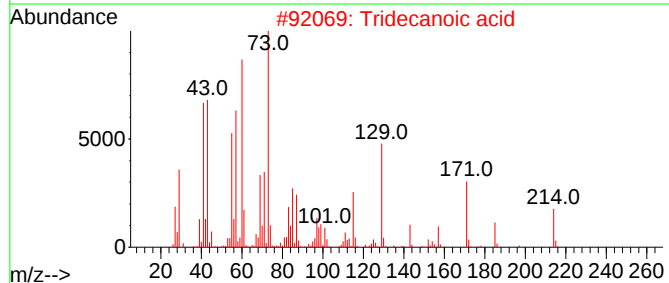
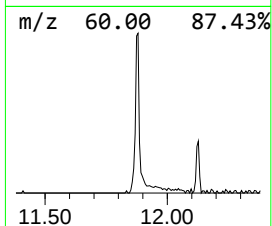
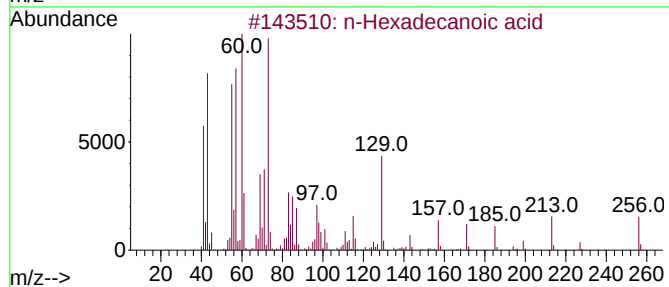
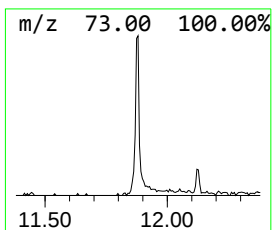
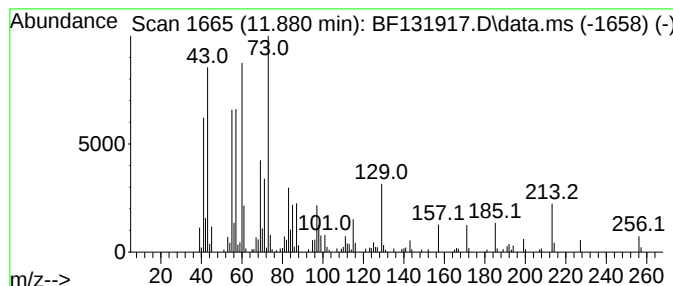
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	5.80 ng	194321	Phenanthrene-d10	11.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	62
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
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Acq On : 05 Jan 2023 16:17
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Sample : 01029-01
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ALS Vial : 5 Sample Multiplier: 1

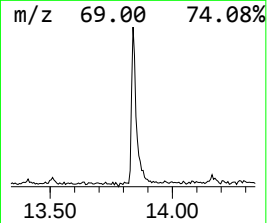
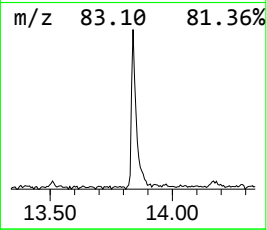
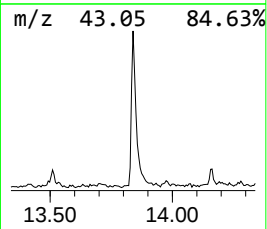
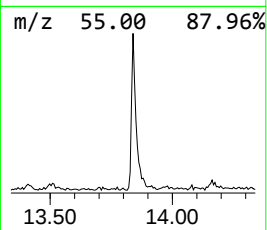
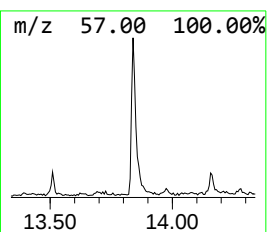
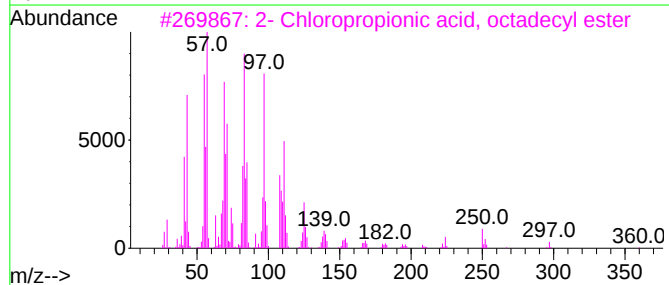
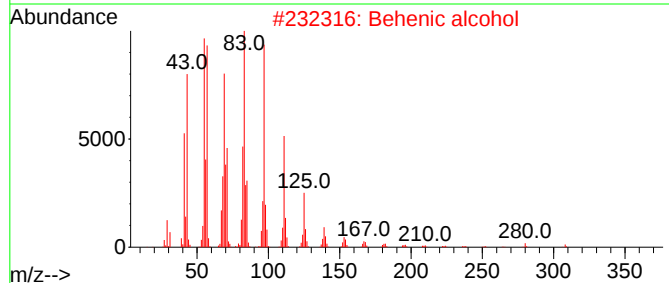
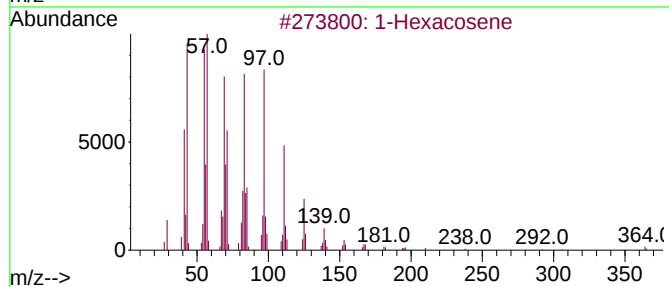
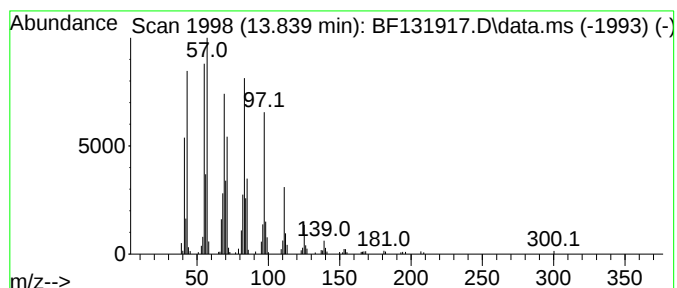
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ClientSampleId :
TP-205

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.839	14.68 ng	298585	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	94
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131917.D
Acq On : 05 Jan 2023 16:17
Operator : CG\JU
Sample : 01029-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-205

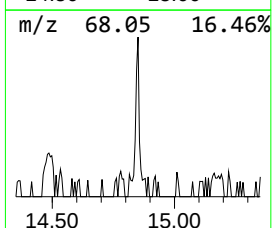
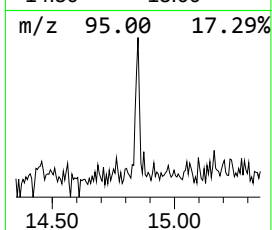
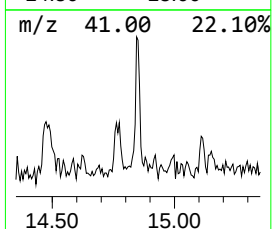
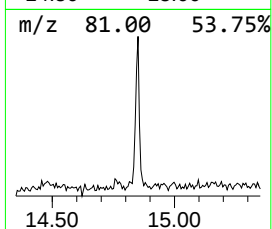
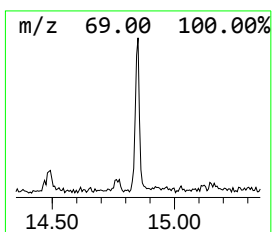
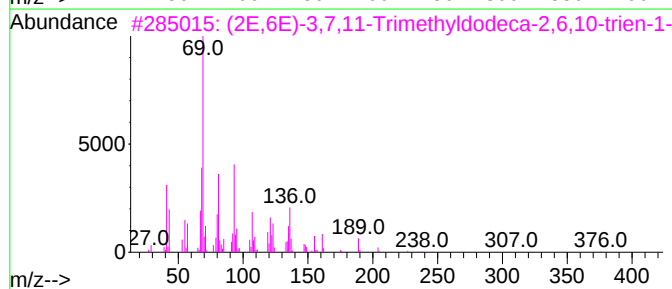
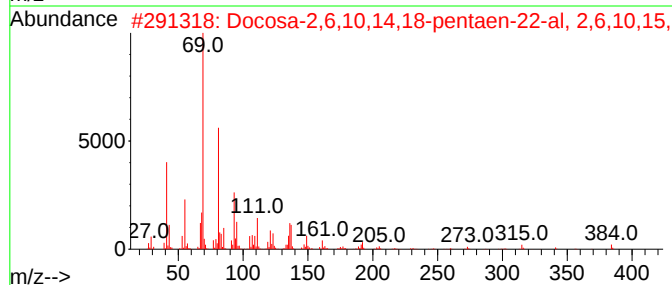
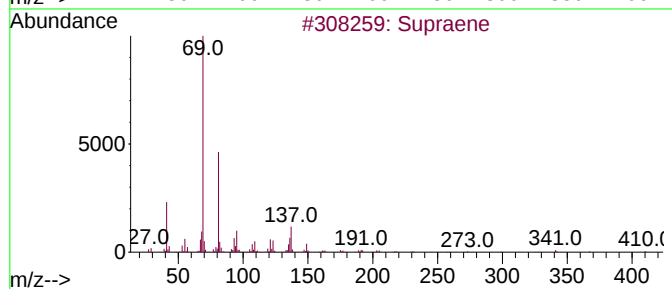
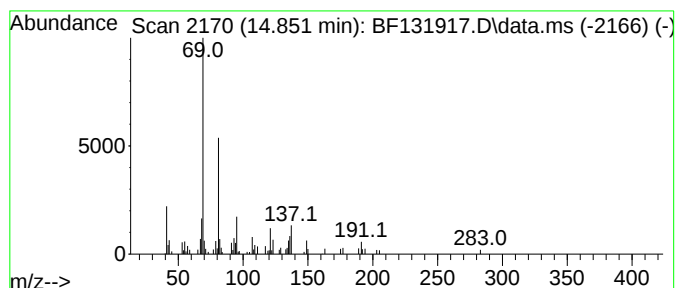
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Supraene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.851	2.20 ng	42258	Perylene-d12	15.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	64
3			(2E,6E)-3,7,11-Trimethyldodeca-2...	376	C25H44O2	078368-57-7	64
4			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	59
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131917.D
Acq On : 05 Jan 2023 16:17
Operator : CG\JU
Sample : 01029-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

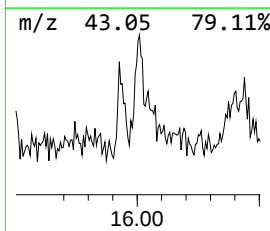
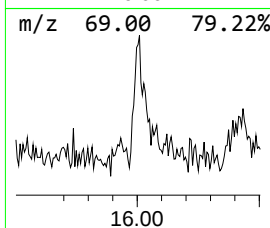
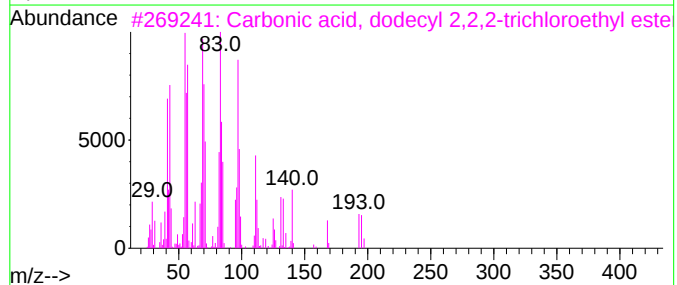
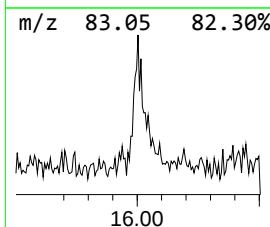
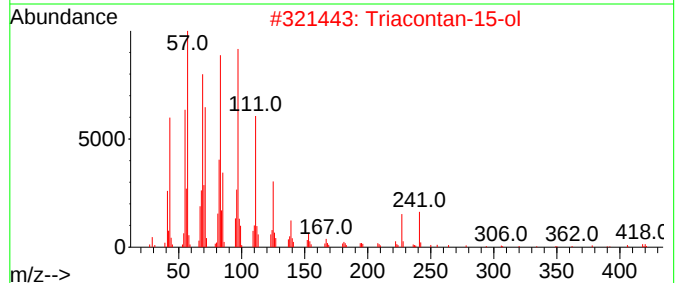
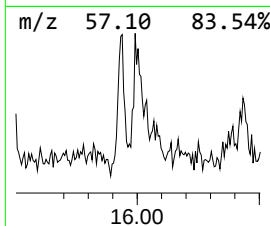
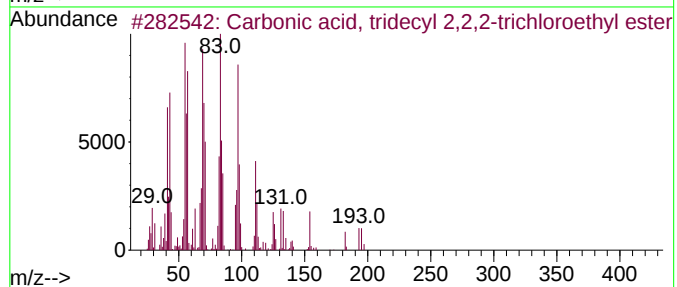
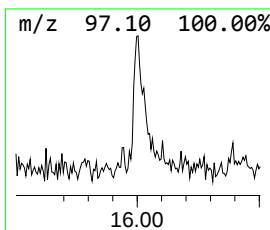
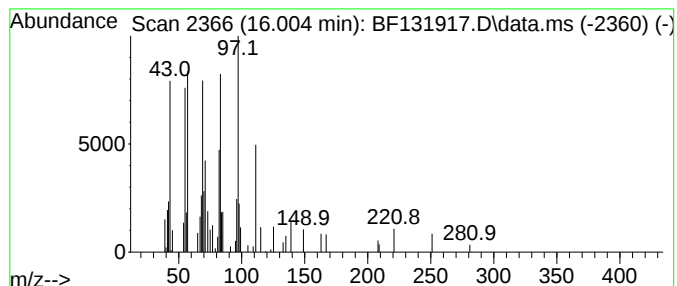
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbonic acid, tridecyl 2,2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.004	3.18 ng	61089	Perylene-d12	15.474	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, tridecyl 2,2,2-tr...	374	C16H29Cl3O3	1000314-55-9	86
2	Triacontan-15-ol	438	C30H62O	031849-26-0	80
3	Carbonic acid, dodecyl 2,2,2-tri...	360	C15H27Cl3O3	1000314-55-8	78
4	1-Hexacosanol	382	C26H54O	000506-52-5	78
5	1-Heptacosanol	396	C27H56O	002004-39-9	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010523\
Data File : BF131917.D
Acq On : 05 Jan 2023 16:17
Operator : CG\JU
Sample : 01029-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-205

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122422.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
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2-Pentanone, 4-...	5.010	43.2	ng	893490	1	6.804	413387	20.0
1,4-Naphthalene...	9.480	2.2	ng	70305	3	9.851	634732	20.0
Juglone	9.992	41.8	ng	1326110	3	9.851	634732	20.0
2,3-Dihydrojuglone	10.363	3.5	ng	112516	3	9.851	634732	20.0
Benzophenone	10.575	17.9	ng	567288	3	9.851	634732	20.0
n-Hexadecanoic ...	11.880	5.8	ng	194321	4	11.345	670182	20.0
1-Hexacosene	13.839	14.7	ng	298585	5	13.998	406835	20.0
Supraene	14.851	2.2	ng	42258	6	15.474	384206	20.0
Carbonic acid, ...	16.004	3.2	ng	61089	6	15.474	384206	20.0