

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
 Data File : BF136458.D
 Acq On : 07 Dec 2023 21:09
 Operator : CG\JU
 Sample : 05599-15
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LKWD-BACKFILL-08

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-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136458.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	15	19	26	rVB	30790	45693	1.86%	0.293%
2	3.346	213	214	222	rBV2	15973	29876	1.22%	0.192%
3	5.040	498	502	508	rVB	57189	64627	2.63%	0.414%
4	5.446	566	571	574	rBV	2130663	2073270	84.49%	13.297%
5	6.445	736	741	744	rBV	2225349	2010653	81.93%	12.895%
6	6.798	797	801	804	rBV	838986	617689	25.17%	3.962%
7	7.357	891	896	899	rBV	1380540	1324781	53.98%	8.497%
8	7.616	936	940	943	rBV	36374	32824	1.34%	0.211%
9	8.075	1014	1018	1021	rBV	971953	765417	31.19%	4.909%
10	8.392	1069	1072	1084	rBV	45740	76612	3.12%	0.491%
11	9.151	1197	1201	1205	rBV	2722491	2453986	100.00%	15.739%
12	9.833	1313	1317	1320	rBV	821536	687513	28.02%	4.409%
13	9.933	1329	1334	1338	rBV	48280	60267	2.46%	0.387%
14	10.622	1447	1451	1461	rBV	1143763	992481	40.44%	6.365%
15	11.322	1567	1570	1574	rBV	681875	536054	21.84%	3.438%
16	11.857	1656	1661	1665	rBV2	68271	70529	2.87%	0.452%
17	12.921	1837	1842	1845	rBV	2113964	1890750	77.05%	12.126%
18	13.833	1990	1997	1999	rBV7	22518	36150	1.47%	0.232%
19	13.880	2001	2005	2013	rVV5	38269	83906	3.42%	0.538%
20	13.974	2017	2021	2025	rBV	685322	601036	24.49%	3.855%
21	14.074	2033	2038	2048	rVB5	115033	254813	10.38%	1.634%
22	14.457	2099	2103	2107	rBV	84412	99913	4.07%	0.641%
23	14.845	2165	2169	2172	rBV	87549	99945	4.07%	0.641%
24	15.286	2240	2244	2251	rVB2	57367	96433	3.93%	0.618%
25	15.457	2268	2273	2278	rBV	396301	497579	20.28%	3.191%
26	15.798	2327	2331	2338	rVB7	48896	89249	3.64%	0.572%

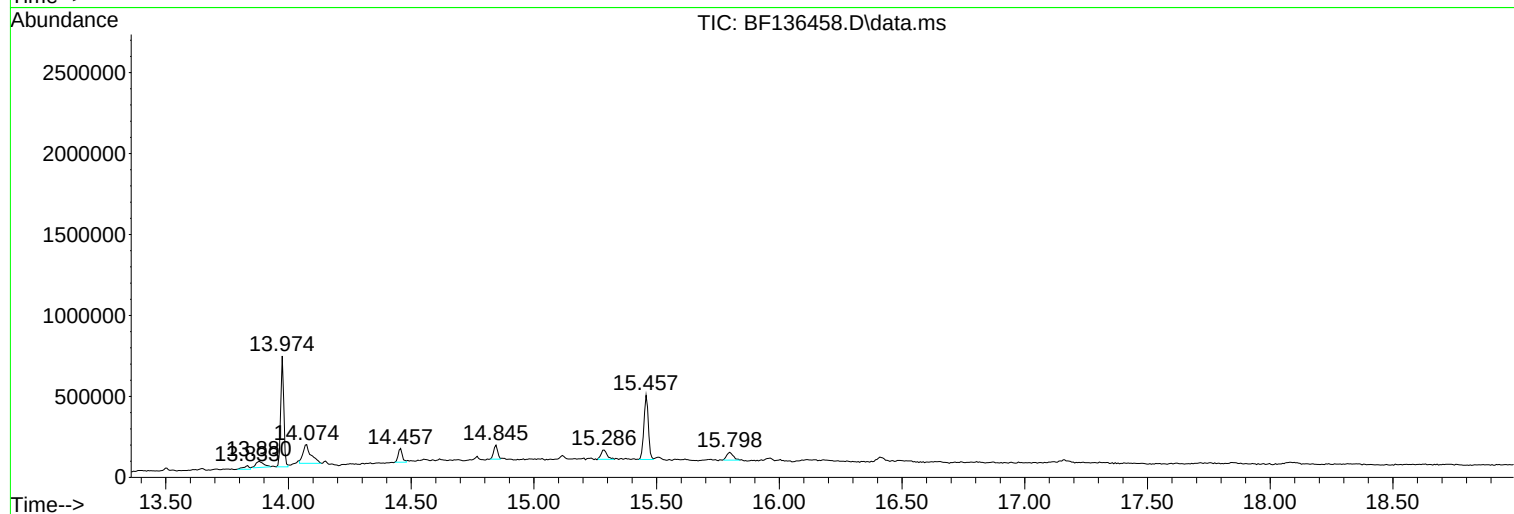
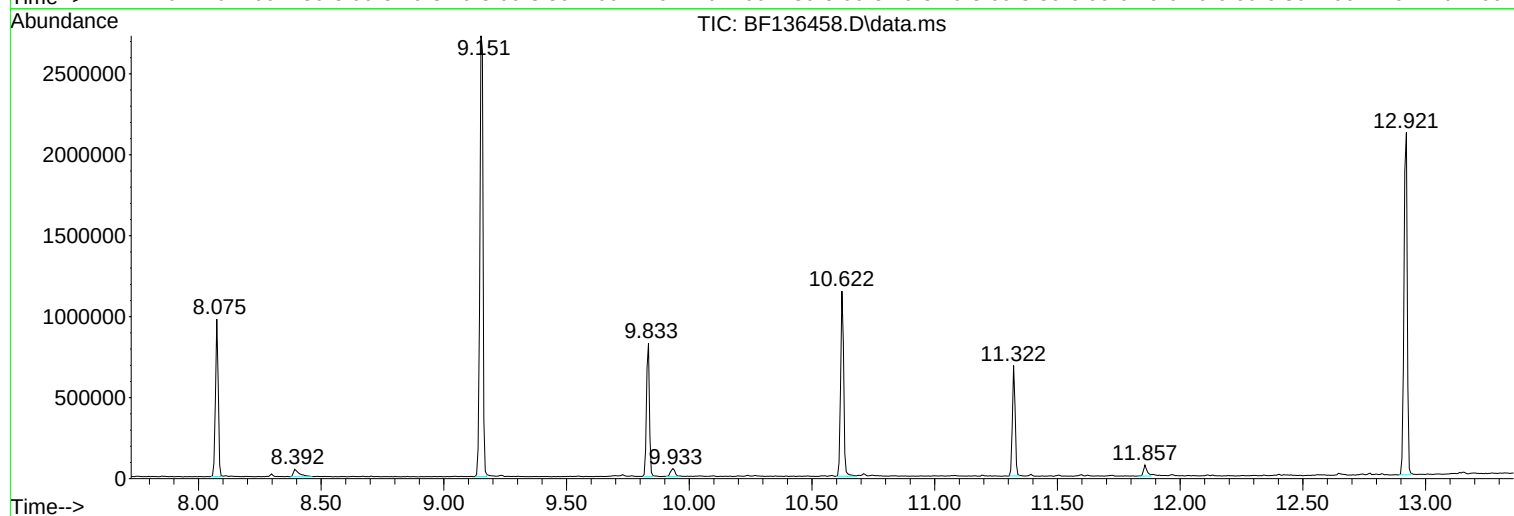
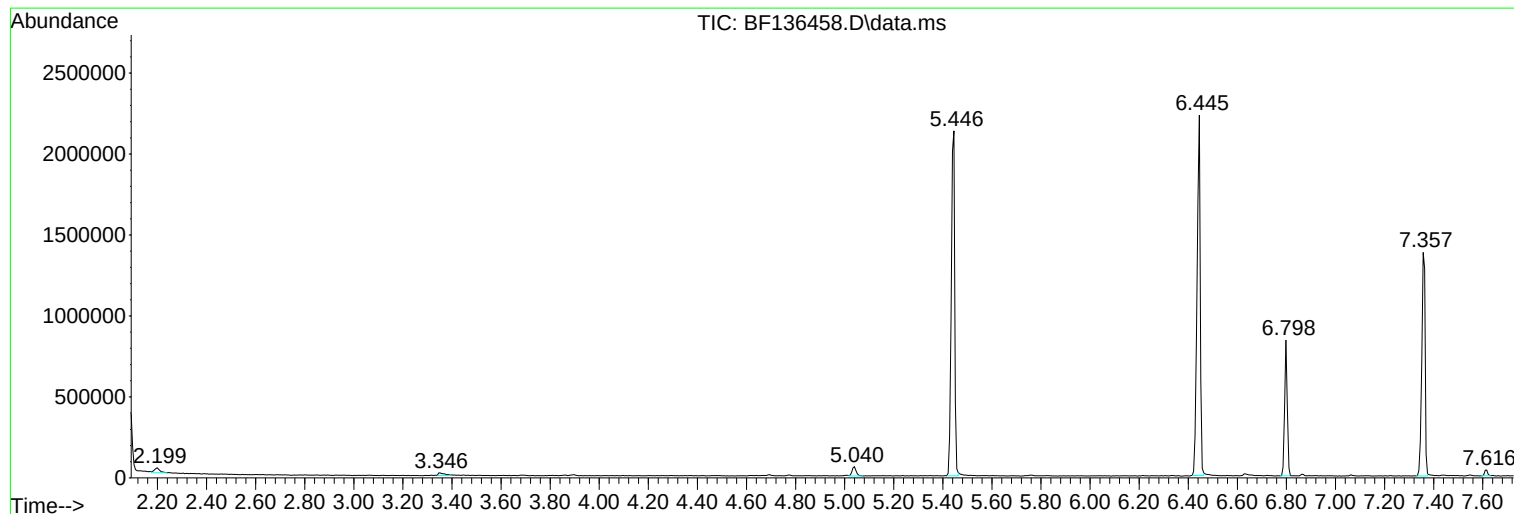
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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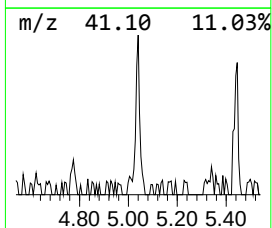
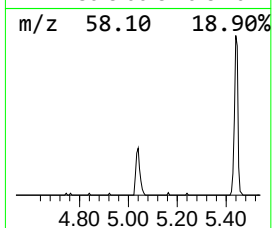
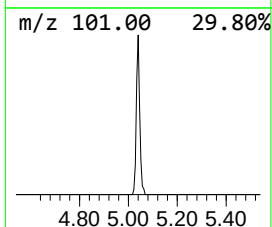
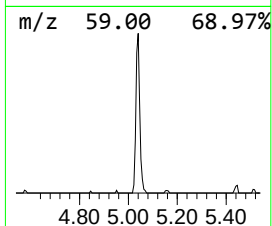
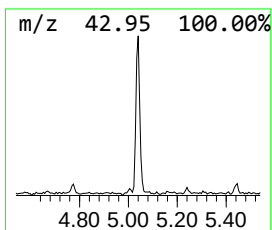
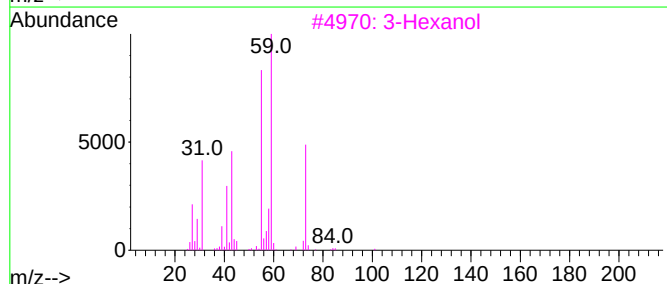
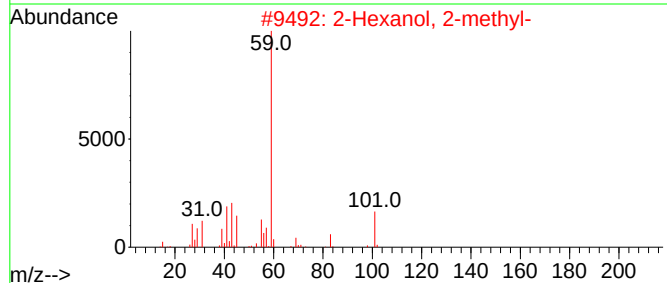
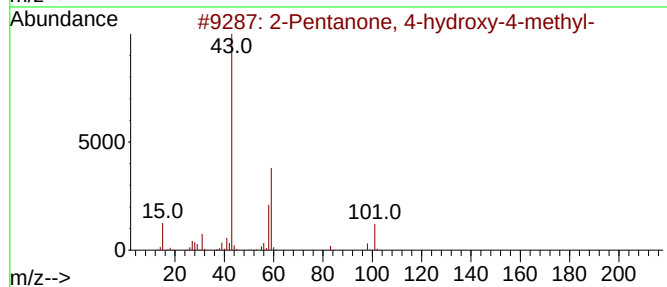
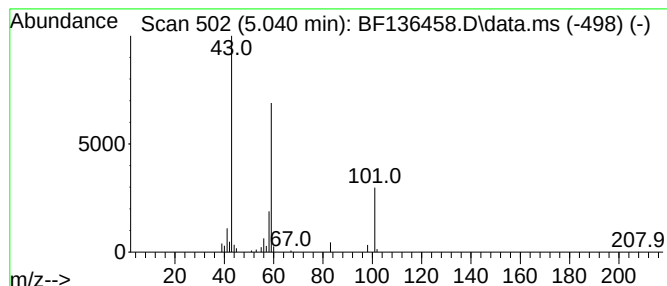
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.09 ng	64627	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3			3-Hexanol	102	C6H14O	000623-37-0	28
4			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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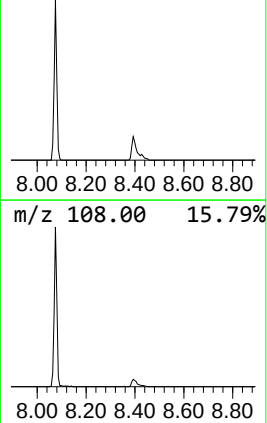
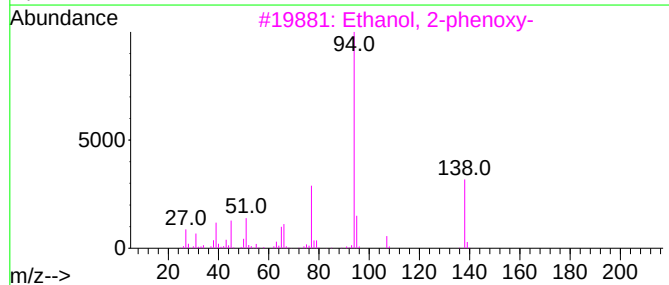
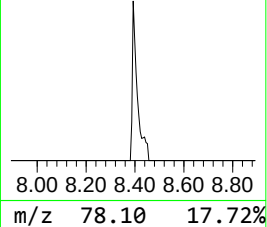
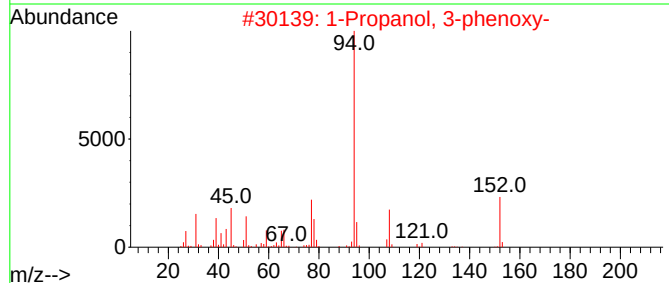
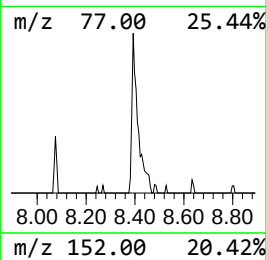
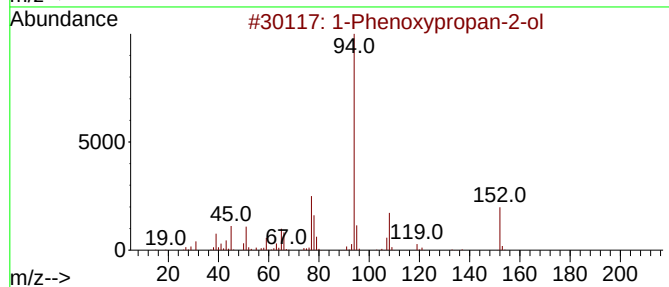
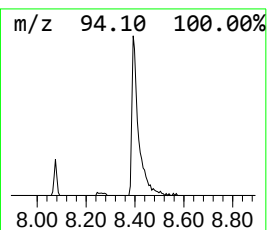
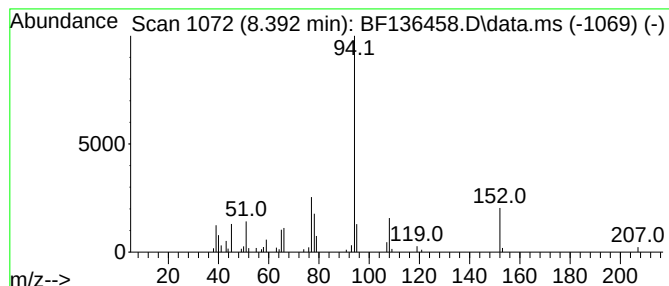
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.392	2.00 ng	76612	Naphthalene-d8	8.075

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2		1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3		Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	59
4		1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5		Benzene, (4-chlorobutoxy)-	184	C10H13ClO	002651-46-9	53



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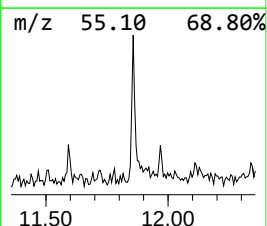
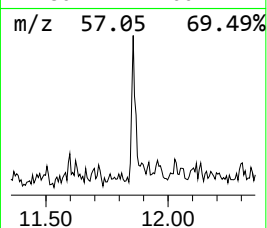
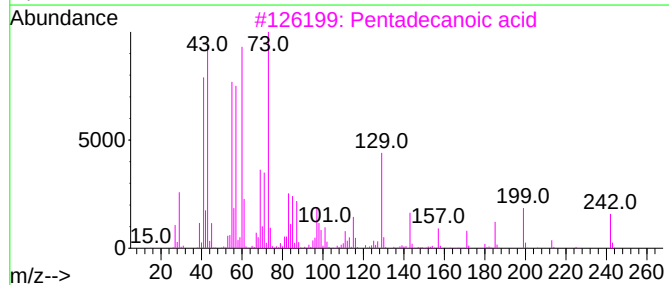
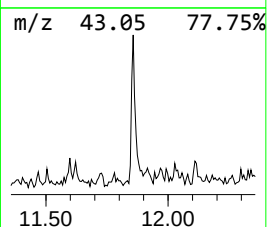
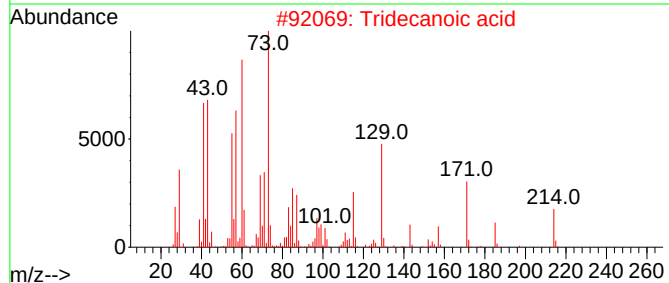
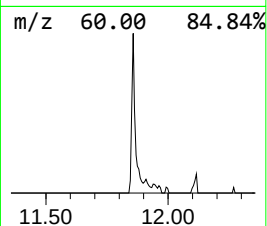
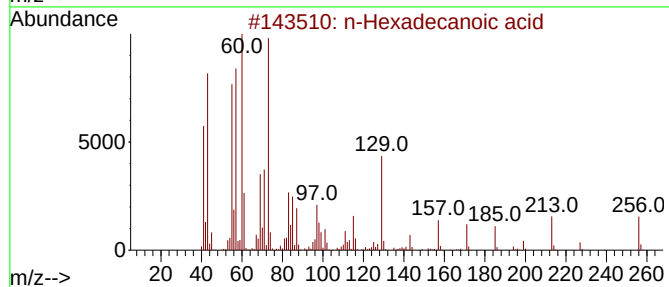
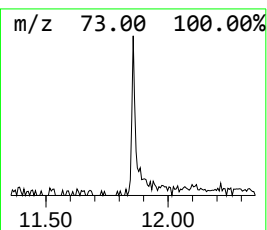
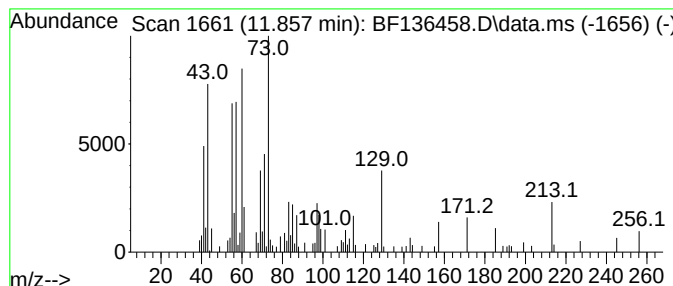
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	2.63 ng	70529	Phenanthrene-d10	11.322

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Trehalose	342	C12H22O11	000099-20-7	35
5			Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	18



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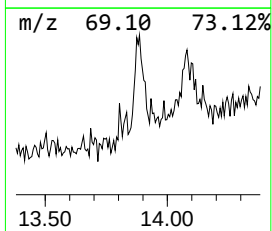
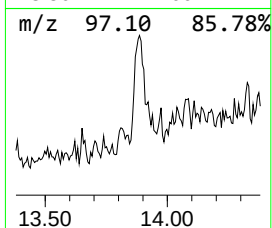
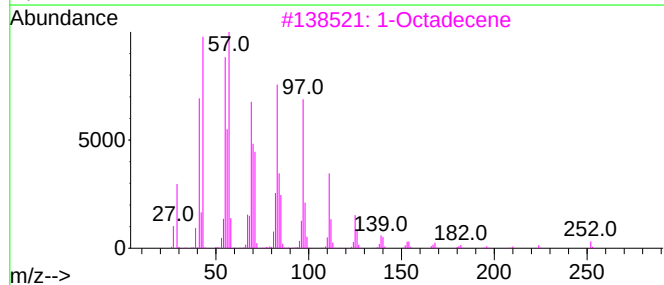
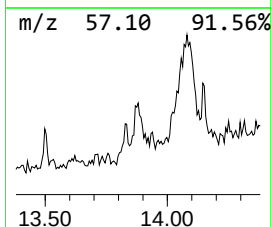
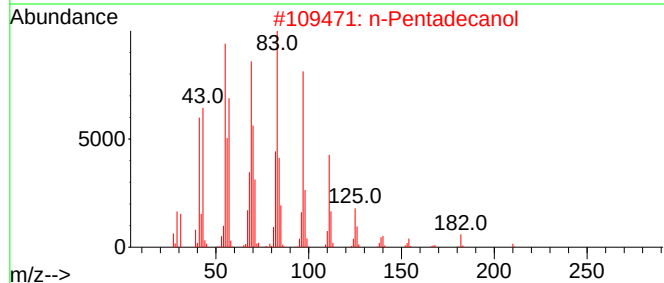
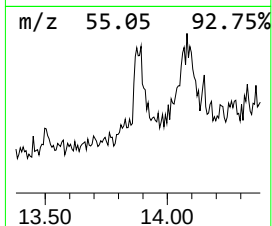
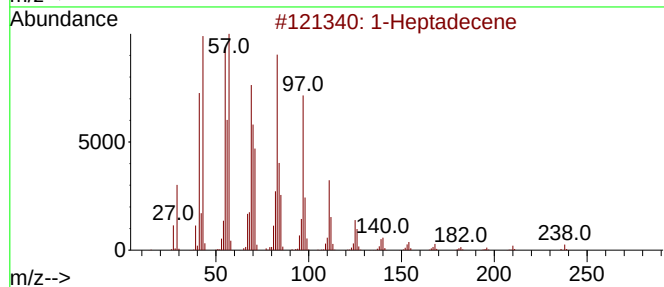
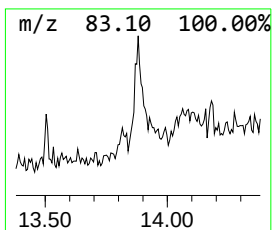
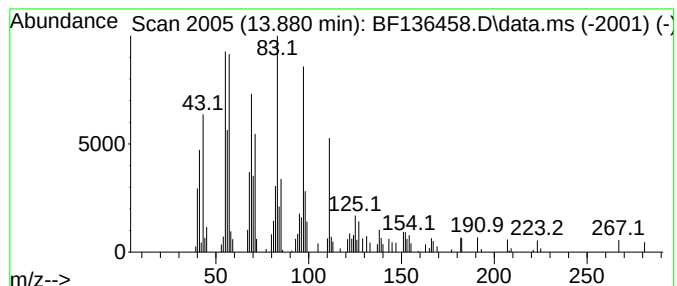
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Peak Number 4 1-Heptadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.79 ng	83906	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	90
2			n-Pentadecanol	228	C15H32O	000629-76-5	80
3			1-Octadecene	252	C18H36	000112-88-9	64
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	58
5			1-Docosene	308	C22H44	001599-67-3	53



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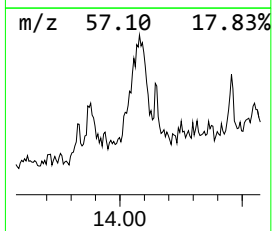
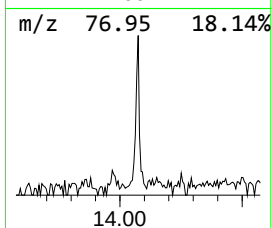
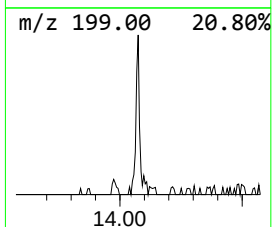
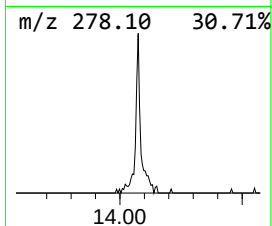
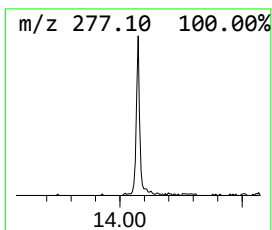
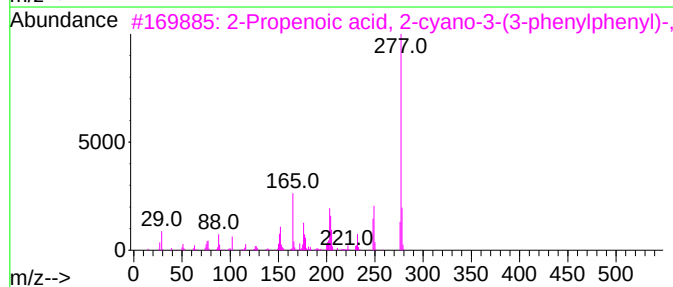
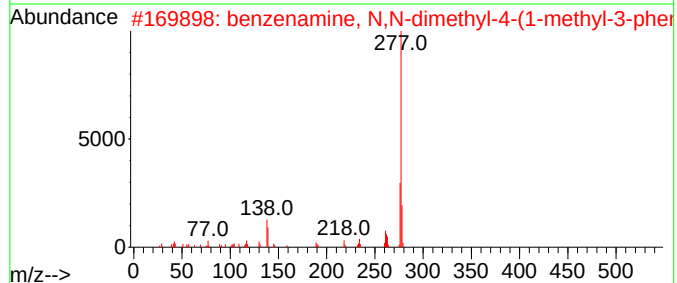
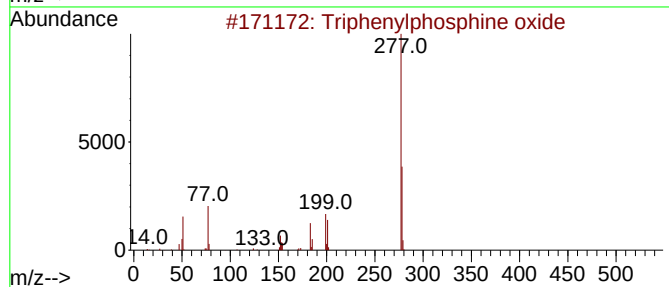
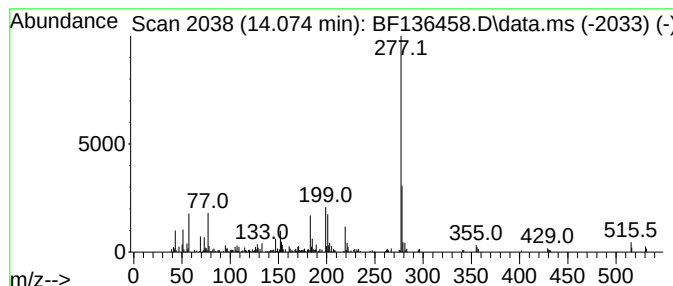
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.074	8.48 ng	254813	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			benzenamine, N,N-dimethyl-4-(1-m...	277	C18H19N3	1000397-11-0	47
3			2-Propenoic acid, 2-cyano-3-(3-p...	277	C18H15NO2	1000080-00-3	47
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	47
5			(Carbethoxymethyl)-triphenylphos...	428	C22H22BrO2P	001530-45-6	42



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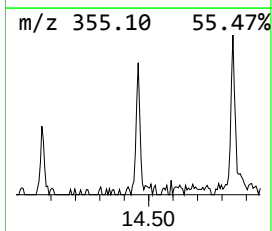
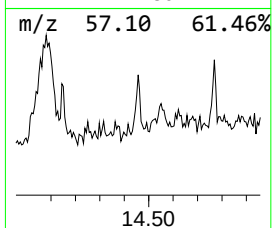
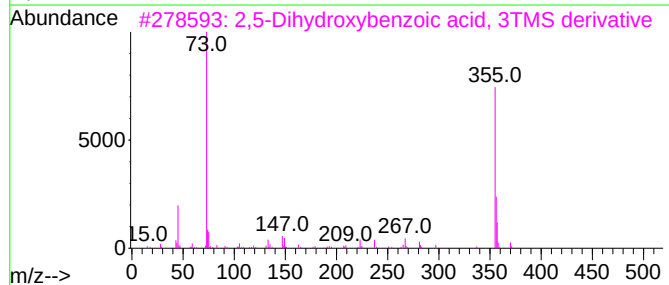
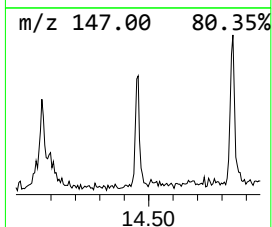
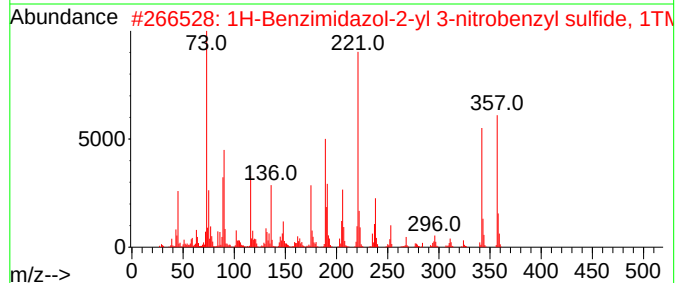
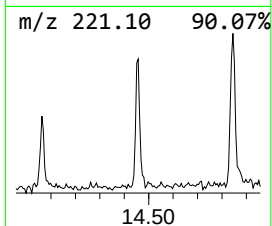
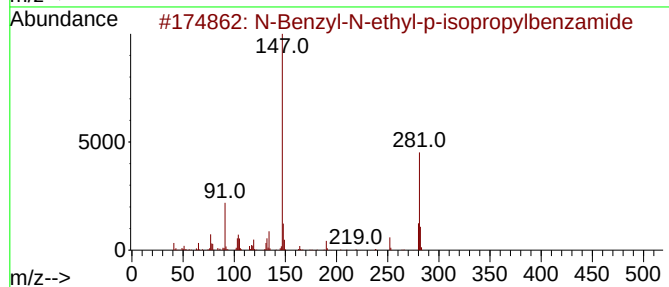
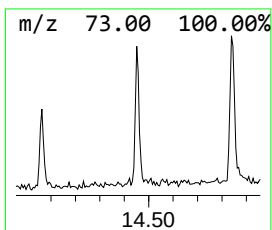
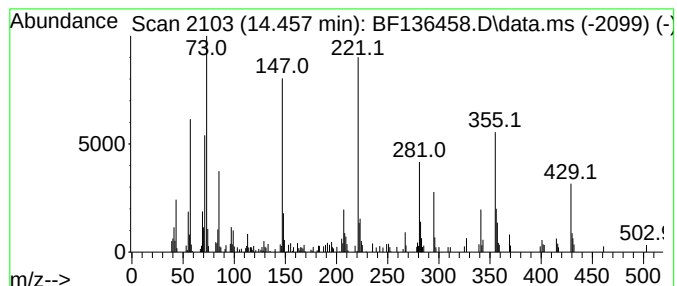
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.457 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.457	3.32 ng	99913	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
2			1H-Benzimidazol-2-yl 3-nitrobenz...	357	C17H19N3O2SSi	1000486-73-3	25
3			2,5-Dihydroxybenzoic acid, 3TMS ...	370	C16H30O4Si3	003618-20-0	25
4			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12
5			Indole, 3-benzoyl-	221	C15H11NO	015224-25-6	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136458.D
Acq On : 07 Dec 2023 21:09
Operator : CG\JU
Sample : 05599-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

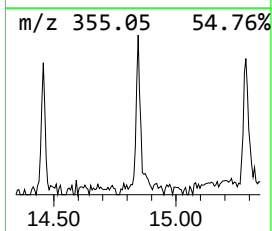
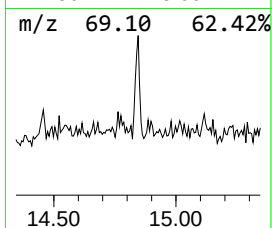
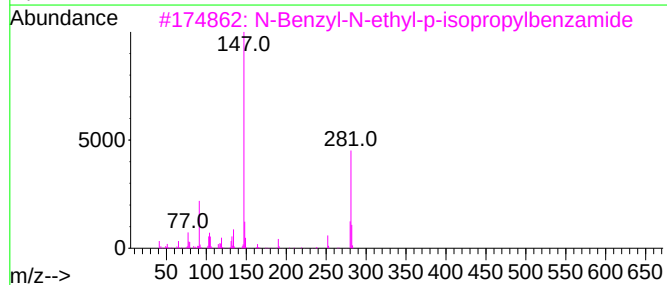
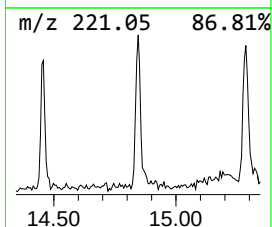
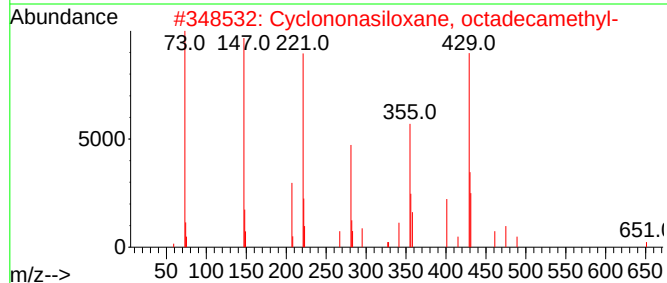
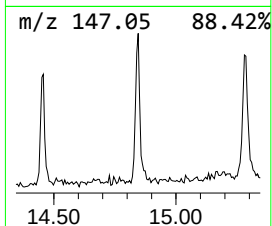
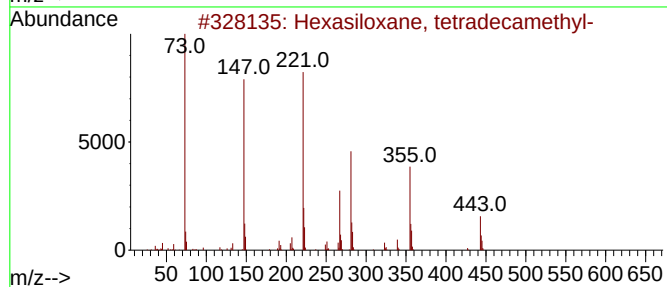
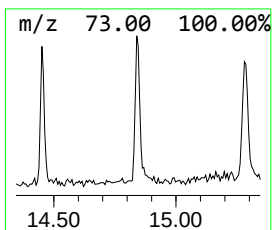
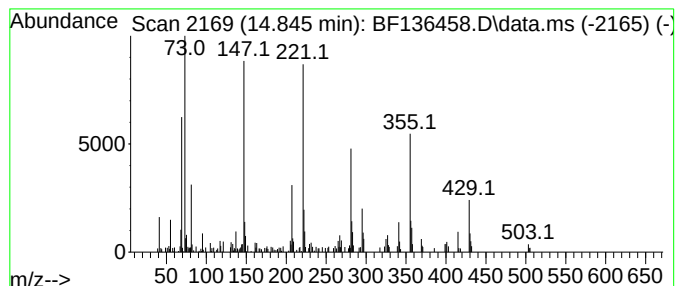
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LKWD-BACKFILL-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexasiloxane, tetradecamethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.845	4.02 ng	99945	Perylene-d12	15.457	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	64
2	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
3	N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	25
4	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	25
5	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136458.D
Acq On : 07 Dec 2023 21:09
Operator : CG\JU
Sample : 05599-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-08

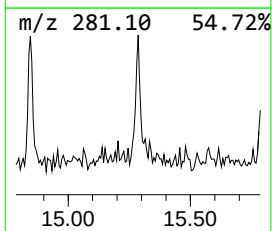
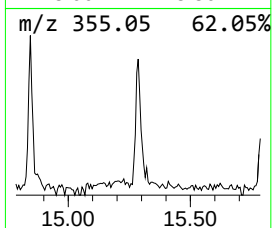
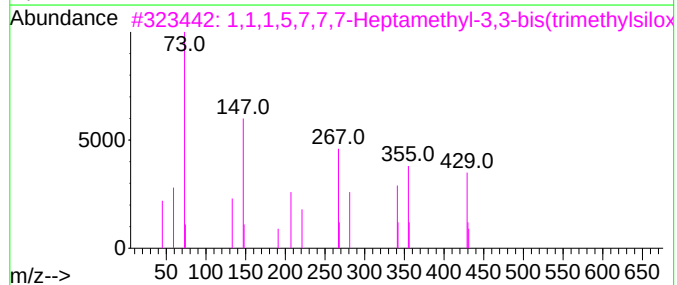
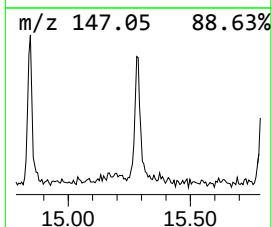
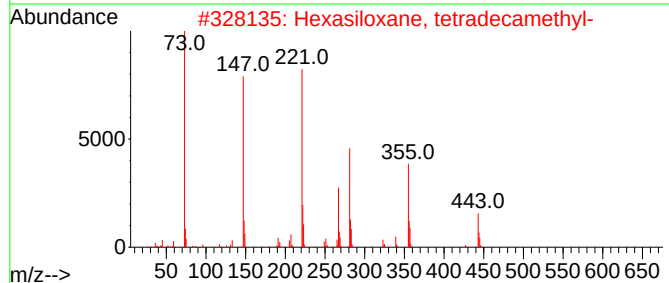
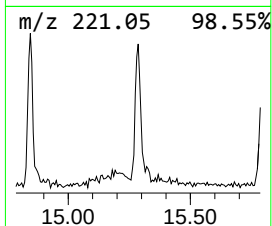
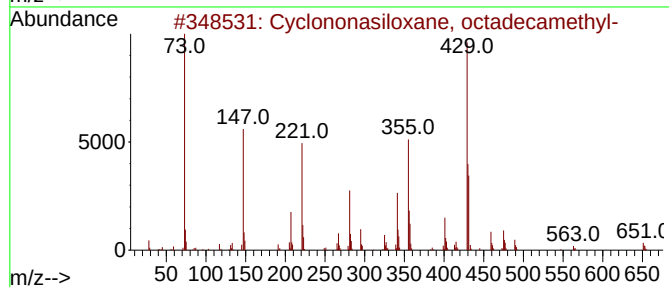
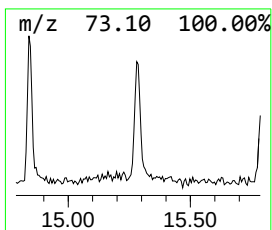
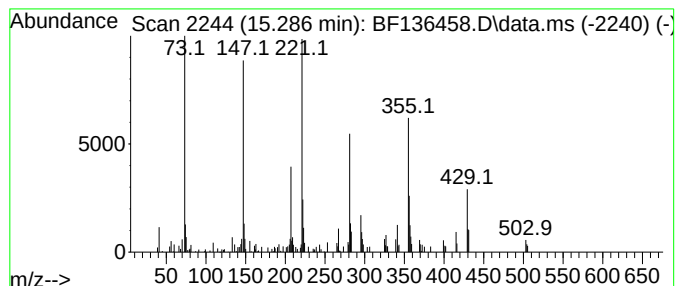
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclononasiloxane, octadeca... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.286	3.88 ng	96433	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	90
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	74
3			1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	40
4			Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	27
5			Mercaptoacetic acid, 2TMS deriva...	236	C8H20O2SSi2	006398-62-5	16



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136458.D
Acq On : 07 Dec 2023 21:09
Operator : CG\JU
Sample : 05599-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-08

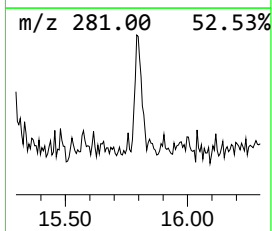
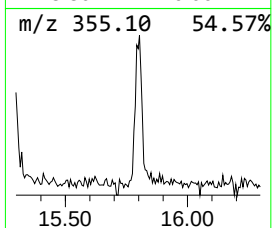
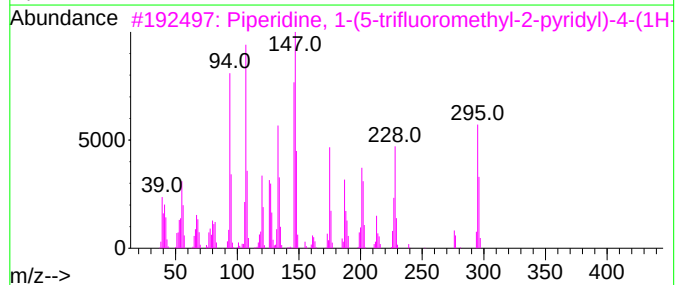
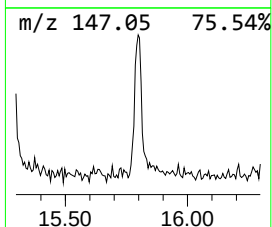
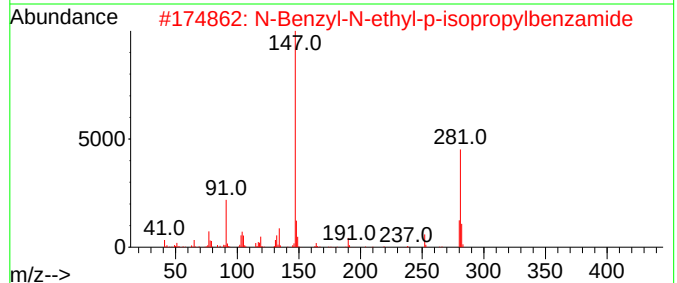
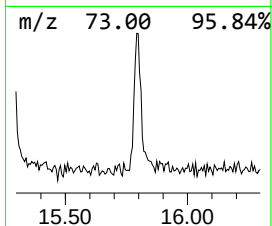
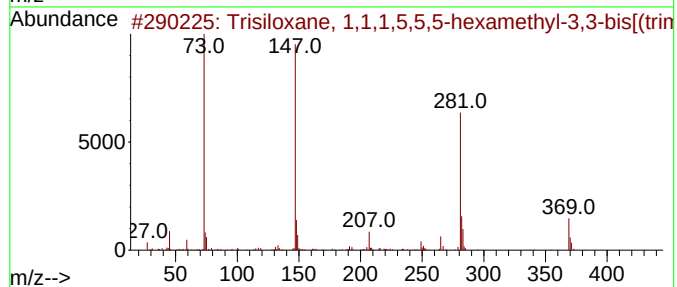
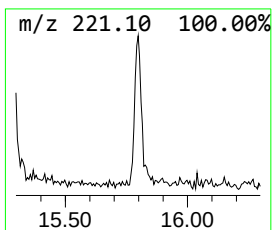
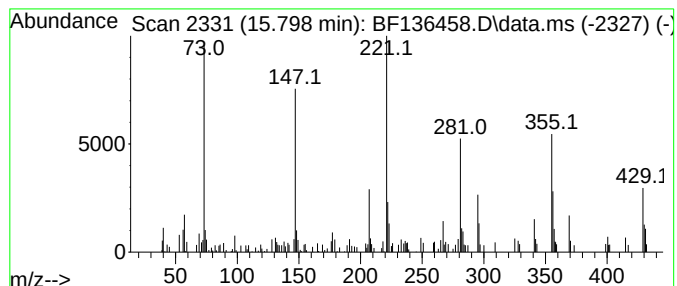
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.798 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.798	3.59 ng	89249	Perylene-d12	15.457

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25
2			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
3			Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	18
4			2,5-Dihydroxybenzoic acid, 3TMS ...	370	C16H30O4Si3	003618-20-0	15
5			1,1,1,3,3,5,5,7,7,9,9,11,11,13,1...	606	C18H54O7Si8	000556-69-4	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF120723\
Data File : BF136458.D
Acq On : 07 Dec 2023 21:09
Operator : CG\JU
Sample : 05599-15
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
LKWD-BACKFILL-08

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.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-...	5.040	2.1	ng	64627	1	6.798	617689	20.0
1-Phenoxypropan...	8.392	2.0	ng	76612	2	8.075	765417	20.0
n-Hexadecanoic ...	11.857	2.6	ng	70529	4	11.322	536054	20.0
1-Heptadecene	13.880	2.8	ng	83906	5	13.974	601036	20.0
Triphenylphosph...	14.074	8.5	ng	254813	5	13.974	601036	20.0
unknown14.457	14.457	3.3	ng	99913	5	13.974	601036	20.0
Hexasiloxane, t...	14.845	4.0	ng	99945	6	15.457	497579	20.0
Cyclononasiloxa...	15.286	3.9	ng	96433	6	15.457	497579	20.0
unknown15.798	15.798	3.6	ng	89249	6	15.457	497579	20.0