

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102023\
 Data File : BF135905.D
 Acq On : 20 Oct 2023 13:28
 Operator : CG\JU
 Sample : PB156209BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB156209BL

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135905.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.357	382	386	403	rBV	62370	116700	4.05%	0.600%
2	4.975	486	491	512	rBV	631845	1010310	35.08%	5.197%
3	5.381	556	560	590	rBV	2522232	2783799	96.67%	14.320%
4	5.757	619	624	632	rBV	23895	30571	1.06%	0.157%
5	6.392	728	732	735	rBV	2407470	2424053	84.18%	12.470%
6	6.733	786	790	803	rVB	546152	515440	17.90%	2.651%
7	7.304	883	887	890	rBV	1629952	1521892	52.85%	7.829%
8	8.010	1004	1007	1022	rBV	750257	676830	23.50%	3.482%
9	9.092	1185	1191	1194	rBV	3165497	2879725	100.00%	14.814%
10	9.769	1302	1306	1318	rVB	876562	744352	25.85%	3.829%
11	10.569	1438	1442	1456	rBV	1798030	1834171	63.69%	9.435%
12	11.268	1557	1561	1569	rBV	790686	719998	25.00%	3.704%
13	11.804	1648	1652	1664	rBV4	17914	40966	1.42%	0.211%
14	12.868	1828	1833	1836	rBV	2858125	2776684	96.42%	14.284%
15	13.933	2010	2014	2023	rBV	591395	571550	19.85%	2.940%
16	14.080	2033	2039	2043	rBV	45044	46791	1.62%	0.241%
17	14.392	2086	2092	2095	rBV	57309	61167	2.12%	0.315%
18	14.692	2137	2143	2147	rBV	56707	65412	2.27%	0.336%
19	15.027	2195	2200	2204	rBV	37863	49658	1.72%	0.255%
20	15.404	2259	2264	2275	rVB	356350	491559	17.07%	2.529%
21	16.992	2528	2534	2545	rVB6	22803	78123	2.71%	0.402%

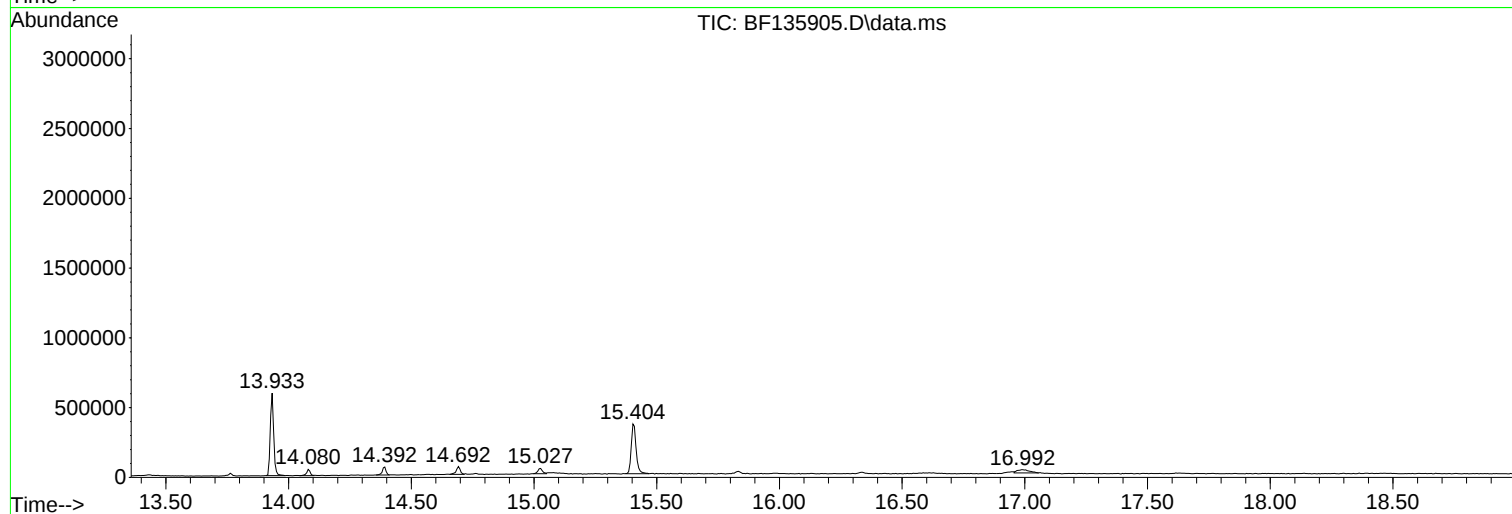
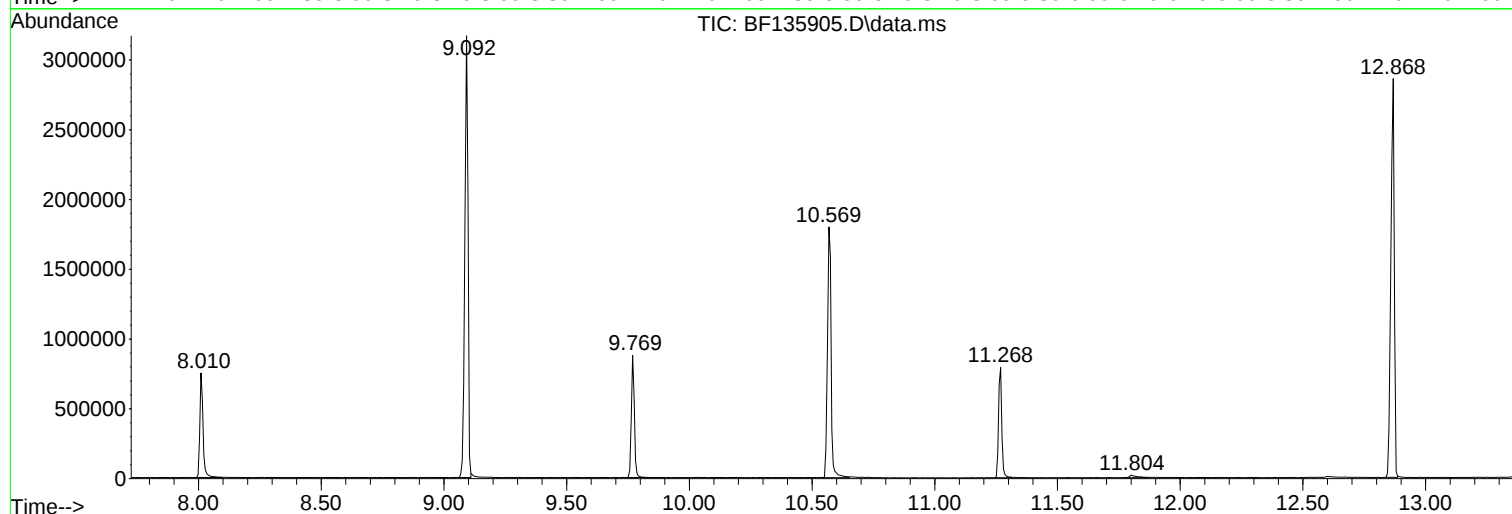
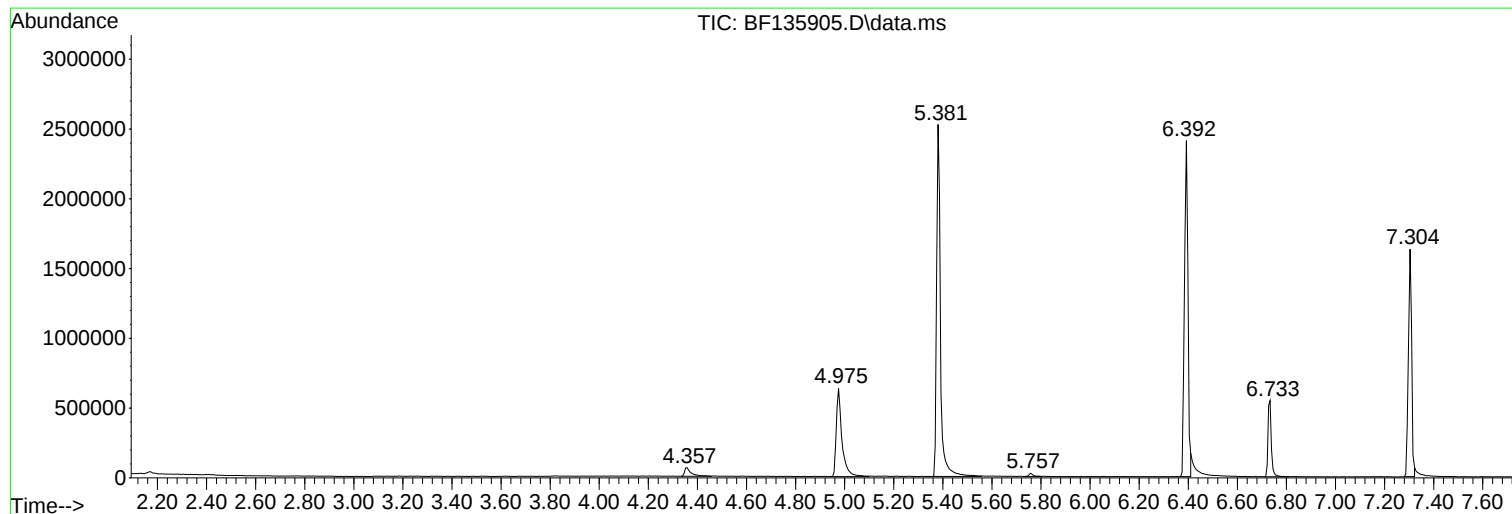
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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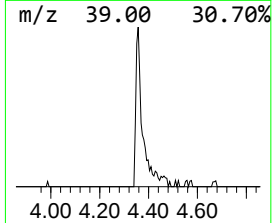
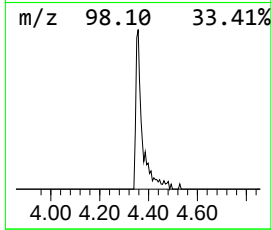
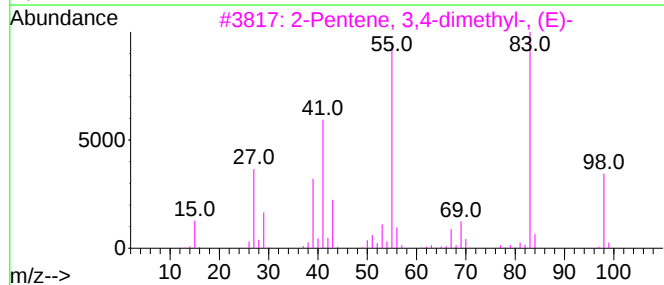
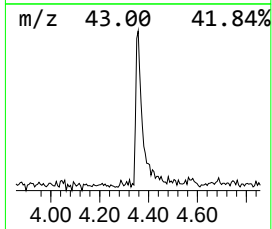
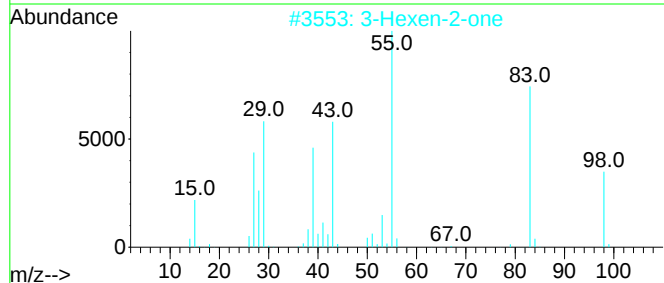
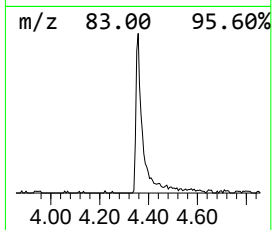
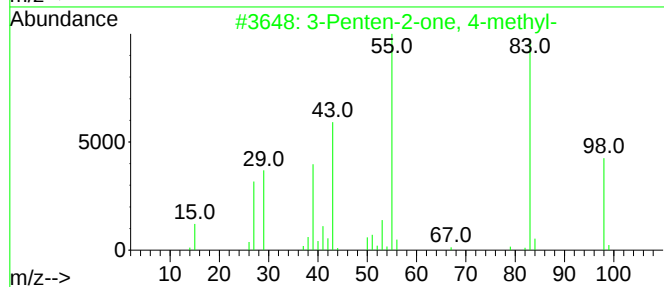
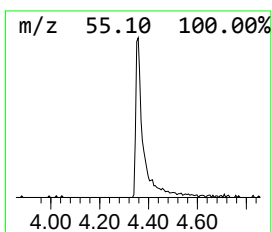
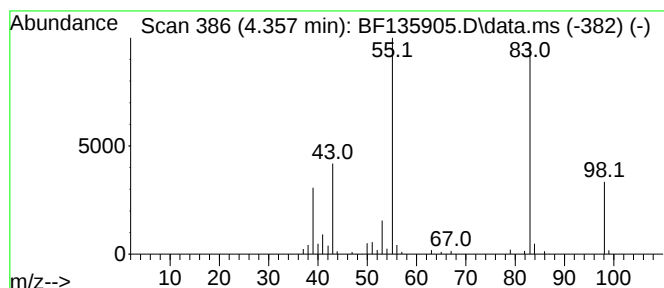
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.357	4.53 ng	116700	1,4-Dichlorobenzene-d4	6.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	91
2	3-Hexen-2-one			98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-			98	C7H14	004914-92-5	80
4	2-Pentene, 3,4-dimethyl-, (Z)-			98	C7H14	004914-91-4	78
5	2-Pentene, 3,4-dimethyl-			98	C7H14	024910-63-2	72



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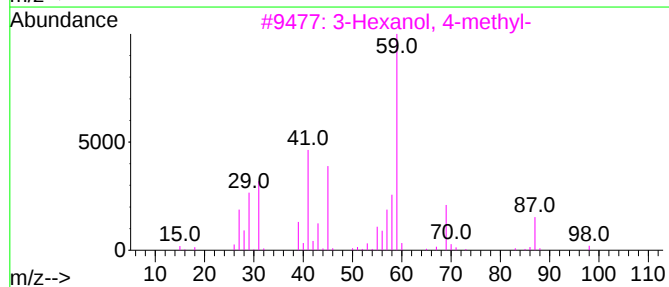
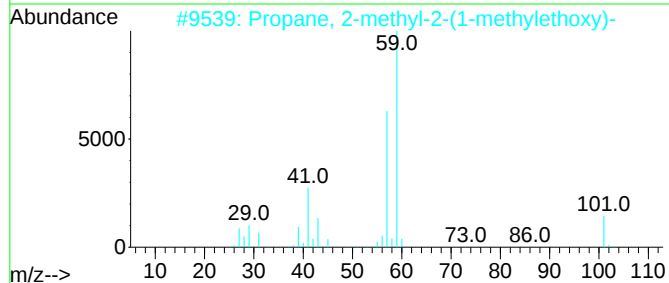
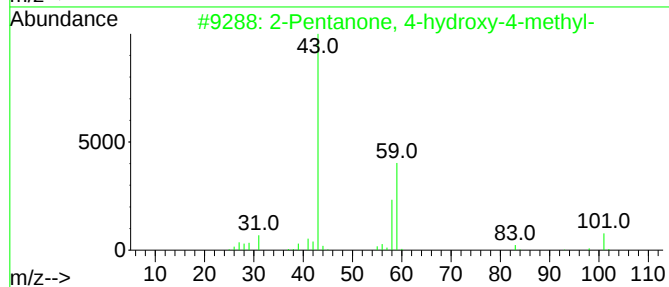
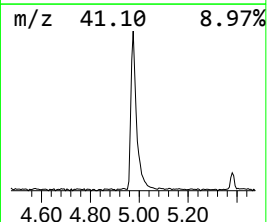
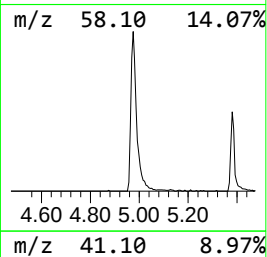
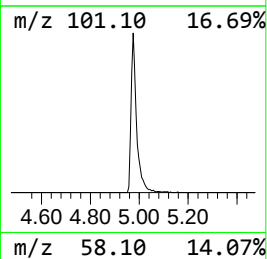
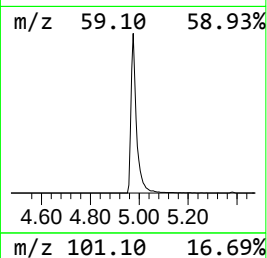
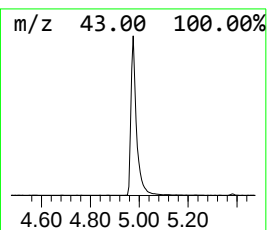
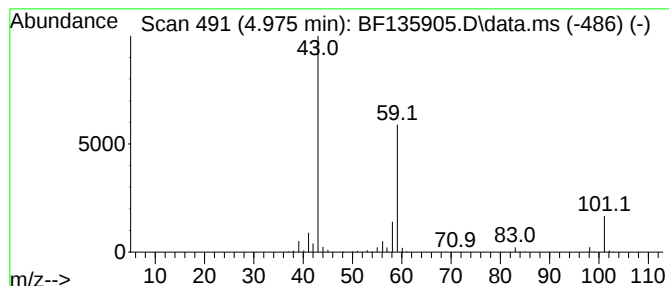
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	39.20 ng	1010310	1,4-Dichlorobenzene-d4	6.733

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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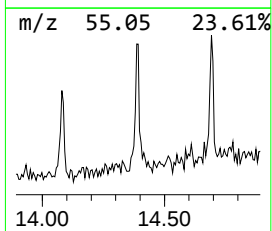
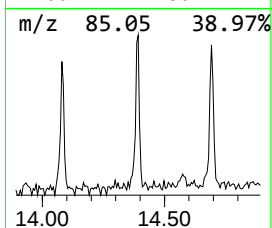
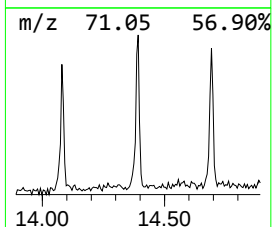
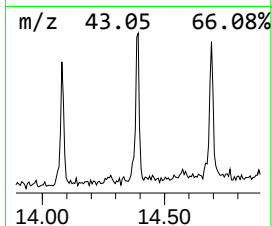
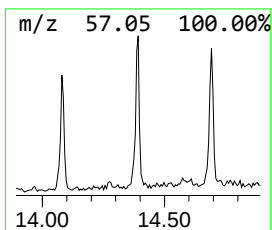
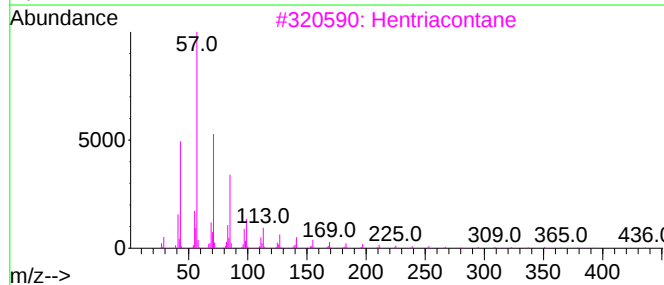
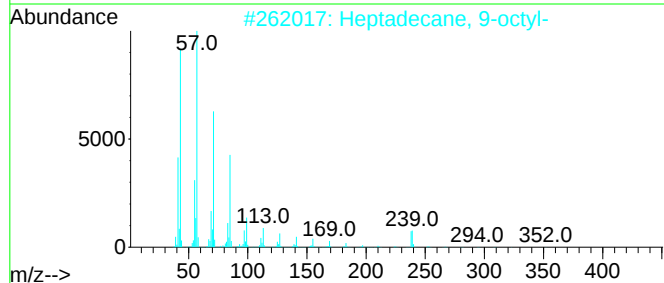
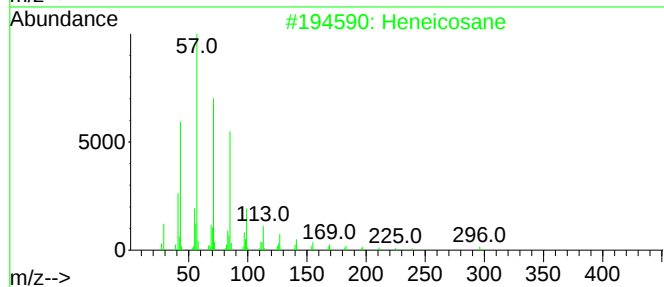
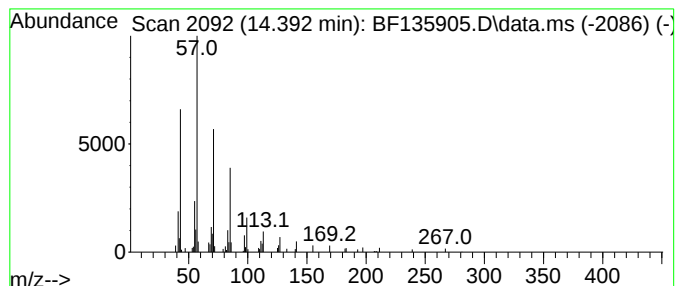
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	2.14 ng	61167	Chrysene-d12	13.933

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



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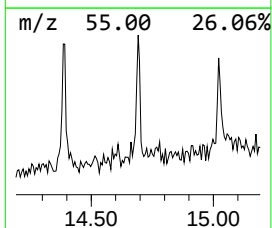
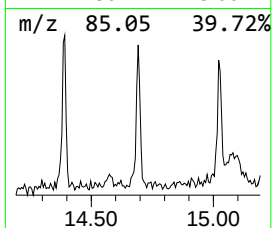
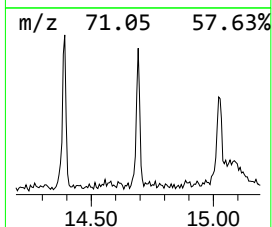
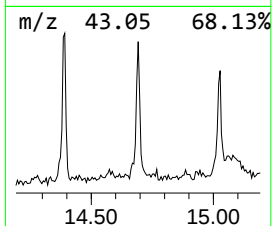
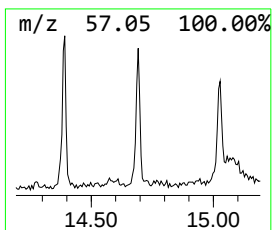
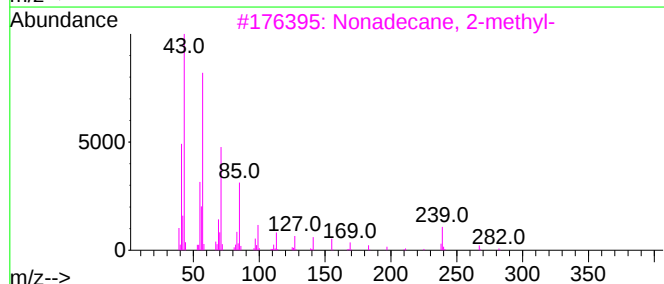
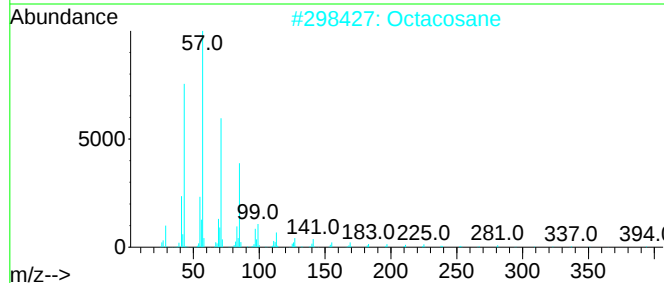
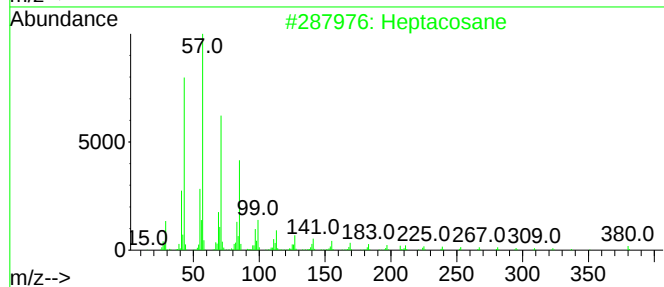
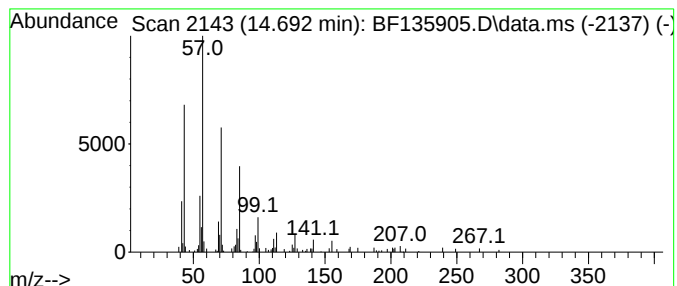
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.692	2.66 ng	65412	Perylene-d12	15.403

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	91
2		Octacosane	394	C28H58	000630-02-4	91
3		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	91
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91



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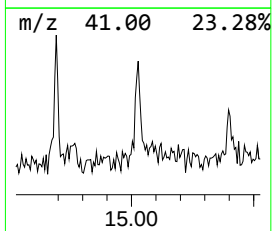
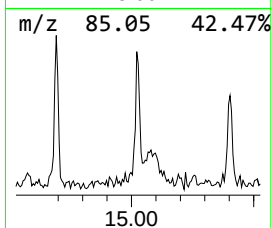
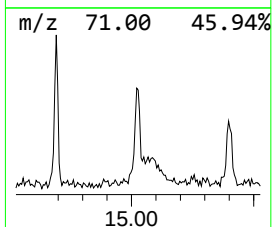
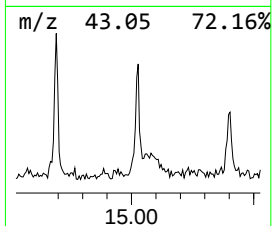
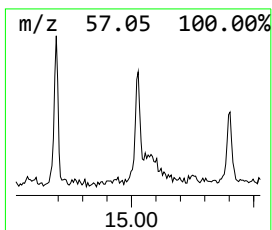
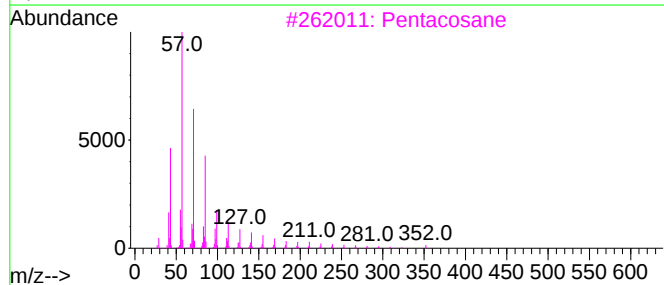
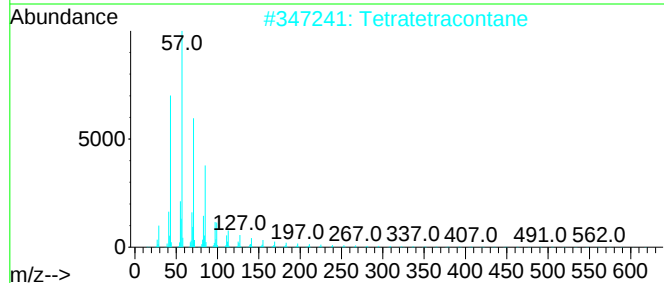
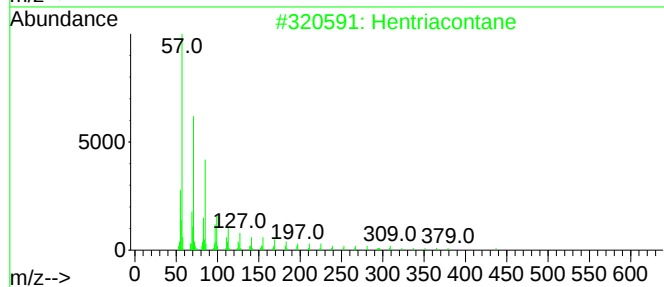
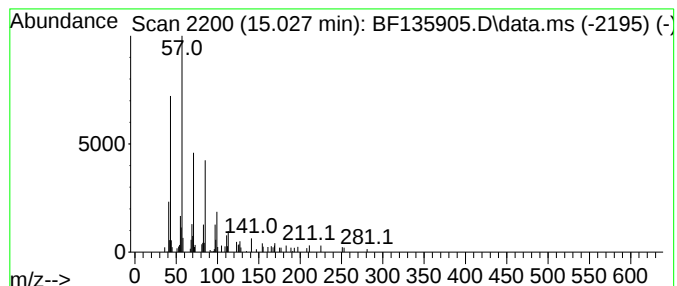
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	2.02 ng	49658	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Pentacosane	352	C25H52	000629-99-2	90
4			Hexatriacontane	507	C36H74	000630-06-8	87
5			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	83



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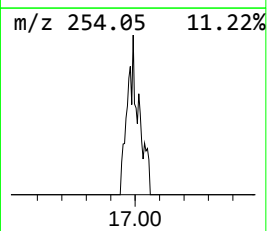
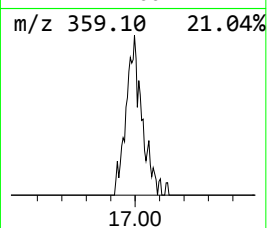
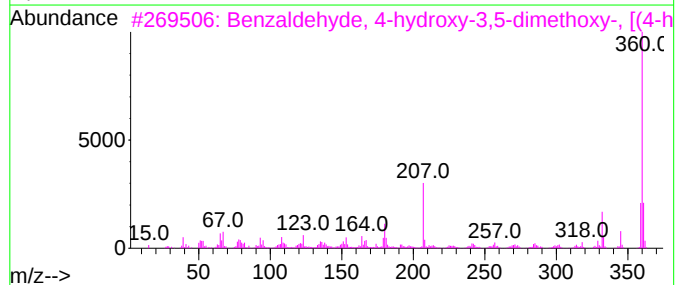
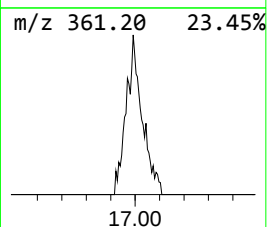
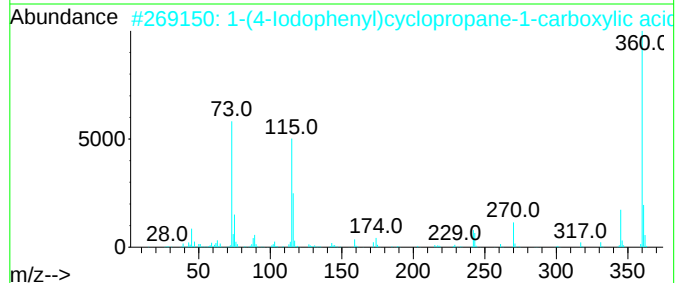
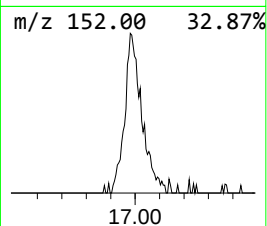
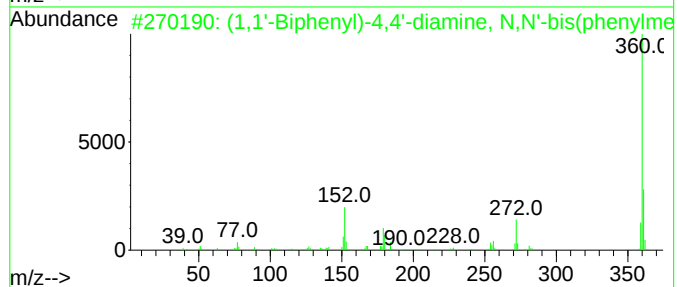
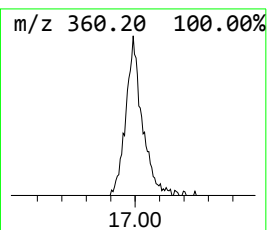
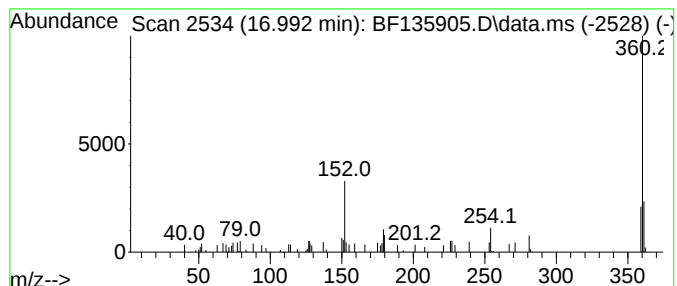
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.992	3.18 ng	78123	Perylene-d12	15.403

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	58
2			1-(4-Iodophenyl)cyclopropane-1-c...	360	C13H17I02Si	1000502-77-3	43
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	40
4			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	40
5			3-Amino-6-nitro-4-phenylsulfanyl...	360	C16H12N2O4S2	1000275-36-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102023\
Data File : BF135905.D
Acq On : 20 Oct 2023 13:28
Operator : CG\JU
Sample : PB156209BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB156209BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.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
3-Penten-2-one,...	4.357	4.5	ng	116700	1	6.733	515440	20.0
2-Pentanone, 4-...	4.975	39.2	ng	1010310	1	6.733	515440	20.0
Heneicosane	14.392	2.1	ng	61167	5	13.933	571550	20.0
Heptacosane	14.692	2.7	ng	65412	6	15.403	491559	20.0
Hentriacontane	15.027	2.0	ng	49658	6	15.403	491559	20.0
(1,1'-Biphenyl)...	16.992	3.2	ng	78123	6	15.403	491559	20.0