

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
 Data File : BF134416.D
 Acq On : 22 Jul 2023 11:46
 Operator : CG\JU
 Sample : PB154316BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154316BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134416.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.498	403	410	413	rBV	1469356	1836188	59.13%	8.132%
2	5.104	505	513	533	rBV	1218508	2011843	64.79%	8.910%
3	5.493	575	579	594	rBV	2348699	2505044	80.67%	11.095%
4	5.863	639	642	647	rBV	78099	68658	2.21%	0.304%
5	6.487	743	748	751	rBV	2305513	2469570	79.53%	10.937%
6	6.840	804	808	817	rBV	533380	450861	14.52%	1.997%
7	7.404	899	904	907	rBV	1540848	1564281	50.38%	6.928%
8	8.116	1021	1025	1032	rBV	741753	599728	19.31%	2.656%
9	9.198	1202	1209	1212	rBV	3220168	2705101	87.12%	11.981%
10	9.875	1321	1324	1328	rBV	784408	630427	20.30%	2.792%
11	10.675	1456	1460	1474	rBV	2036957	1958299	63.07%	8.673%
12	11.375	1575	1579	1582	rBV	824302	700013	22.54%	3.100%
13	12.974	1846	1851	1854	rBV	3273843	3105187	100.00%	13.753%
14	14.039	2028	2032	2037	rBV	666869	614525	19.79%	2.722%
15	14.486	2104	2108	2114	rBV2	44914	72845	2.35%	0.323%
16	14.815	2160	2164	2168	rBV	45176	52351	1.69%	0.232%
17	14.874	2171	2174	2180	rVB2	53951	71633	2.31%	0.317%
18	15.163	2220	2223	2228	rVB	62408	70128	2.26%	0.311%
19	15.315	2245	2249	2254	rBV3	44531	67183	2.16%	0.298%
20	15.551	2283	2289	2295	rBV	398123	617701	19.89%	2.736%
21	16.015	2364	2368	2375	rVB	74481	120668	3.89%	0.534%
22	16.439	2436	2440	2449	rVB	24261	58151	1.87%	0.258%
23	16.557	2455	2460	2465	rVB	58731	101242	3.26%	0.448%
24	17.186	2561	2567	2574	rBV5	53350	127340	4.10%	0.564%

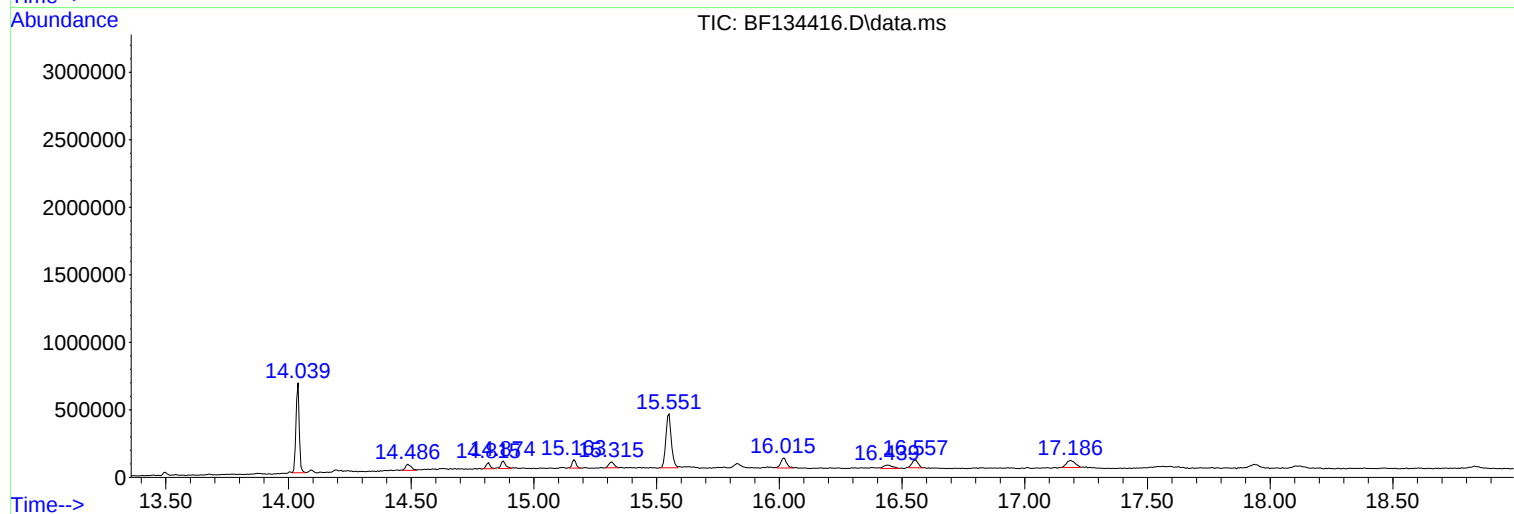
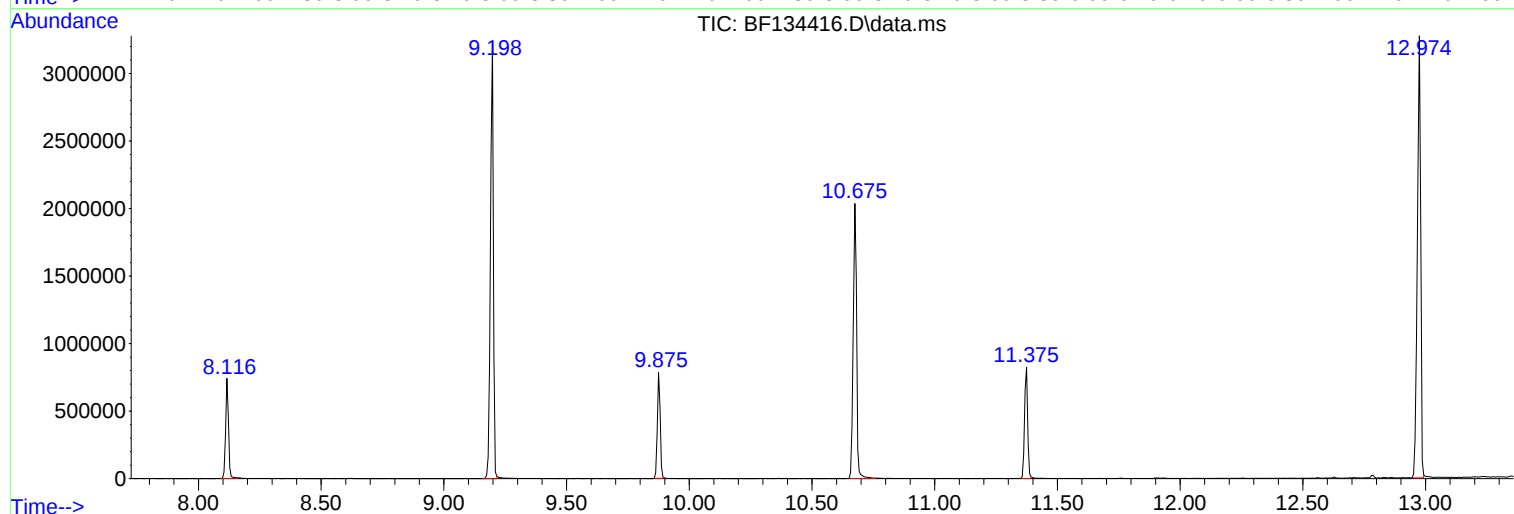
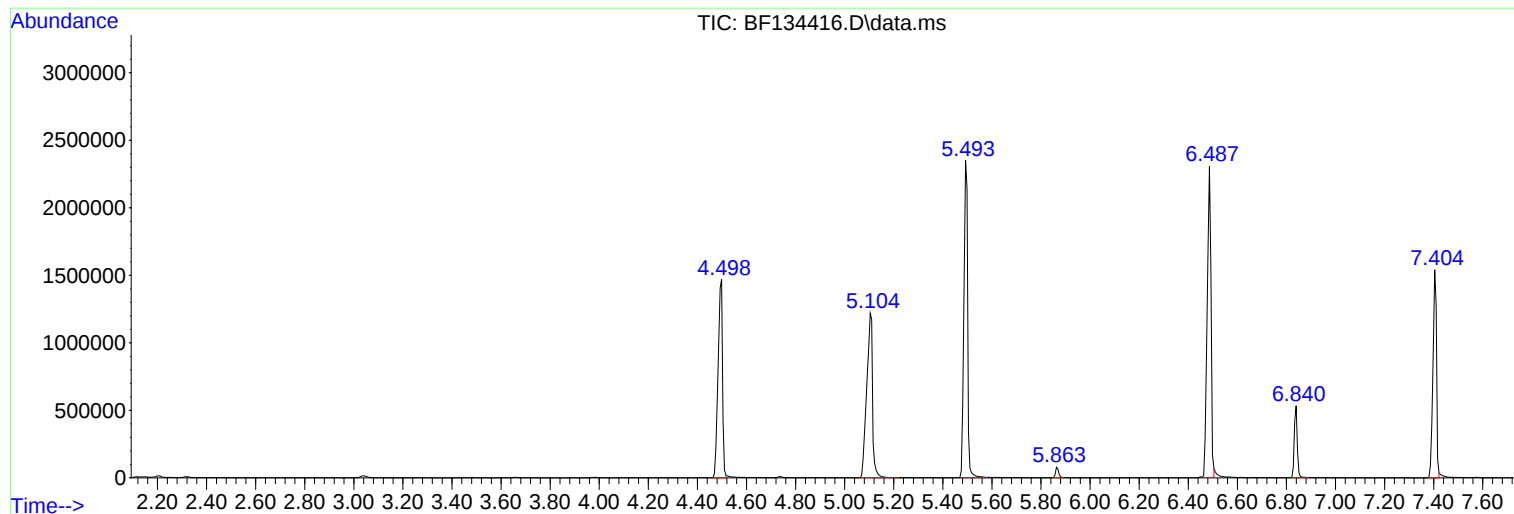
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Instrument :
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ClientSampleId :
PB154316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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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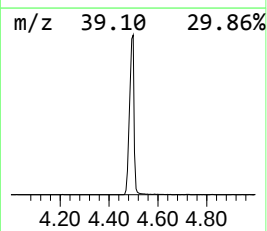
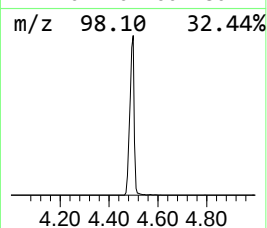
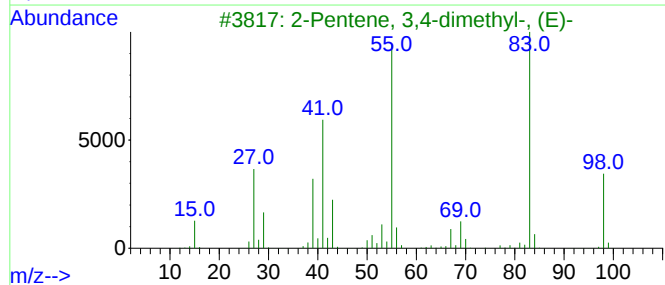
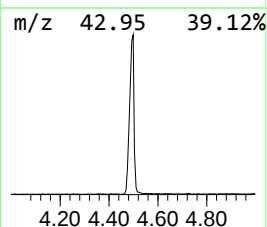
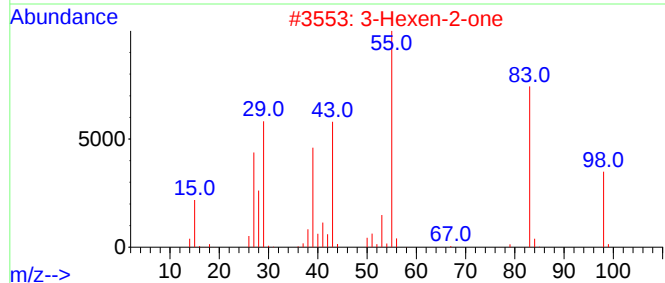
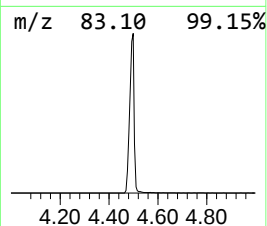
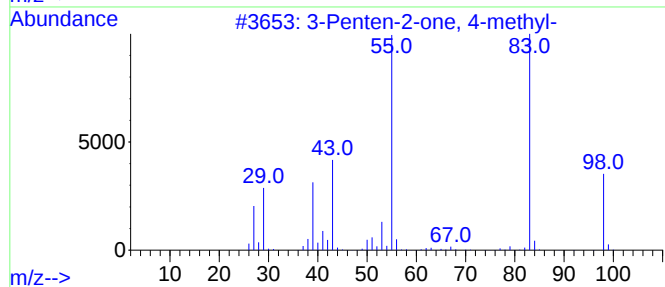
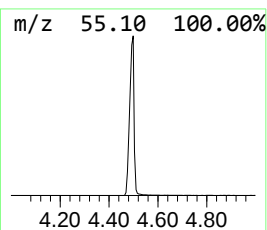
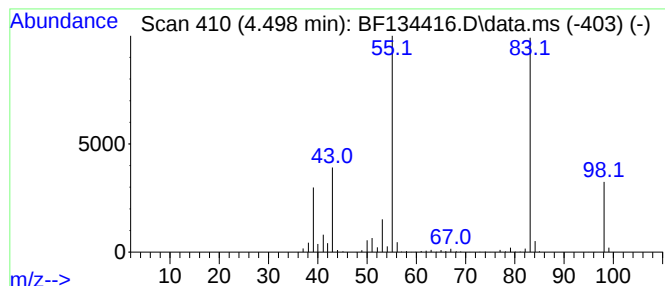
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.498	81.45 ng	1836190	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-			98	C6H10O	000141-79-7	95
2	3-Hexen-2-one			98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-			98	C7H14	004914-92-5	90
4	2-Pentene, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-			98	C7H14	000625-65-0	86



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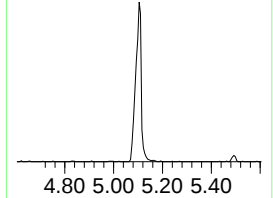
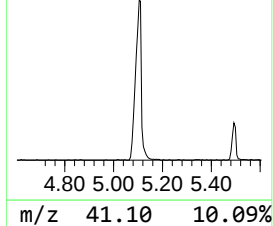
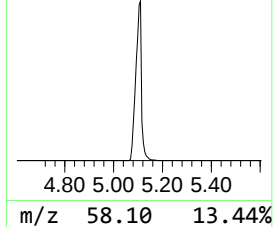
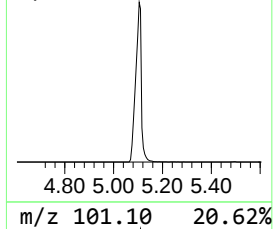
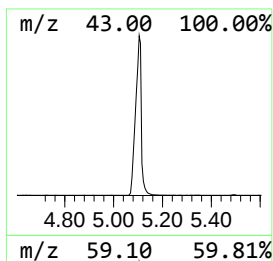
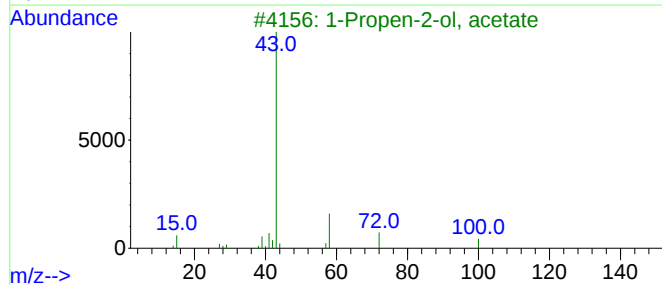
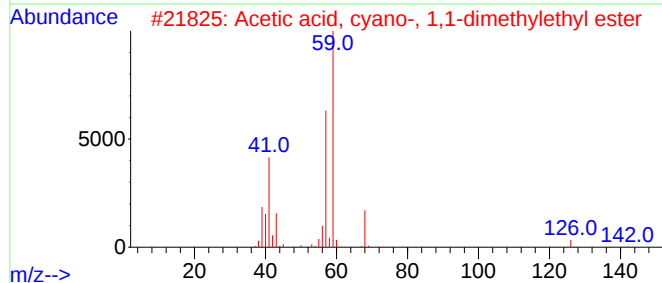
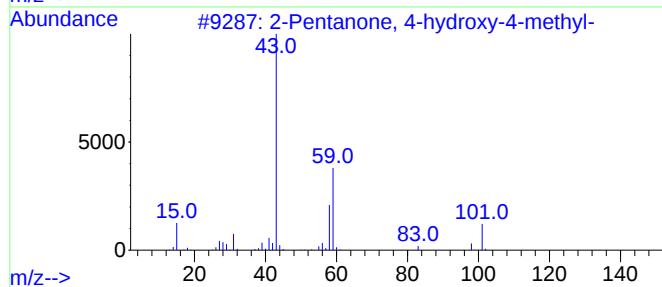
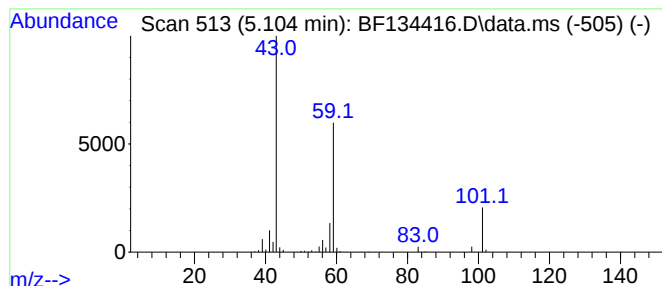
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.104	89.24 ng	2011840	1,4-Dichlorobenzene-d4			6.840
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	23
3	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
4	4-Penten-2-one, 4-methyl-		98	C6H10O	003744-02-3	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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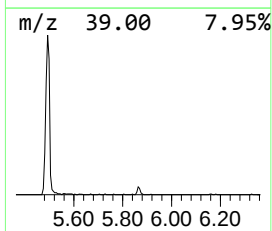
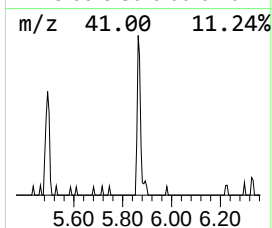
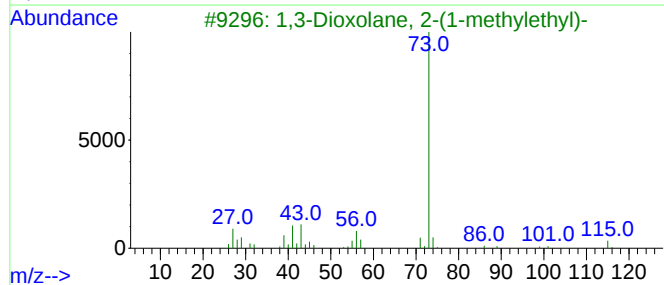
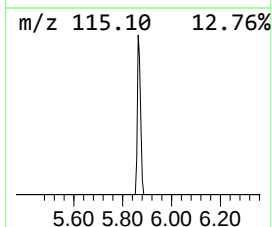
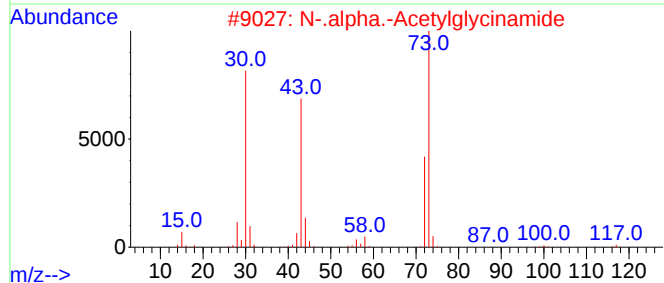
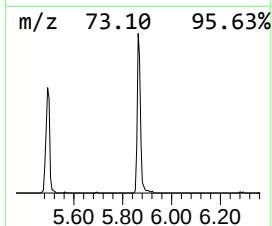
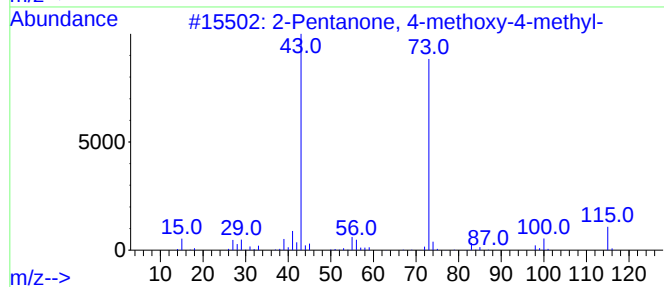
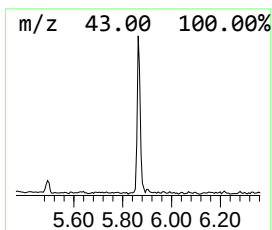
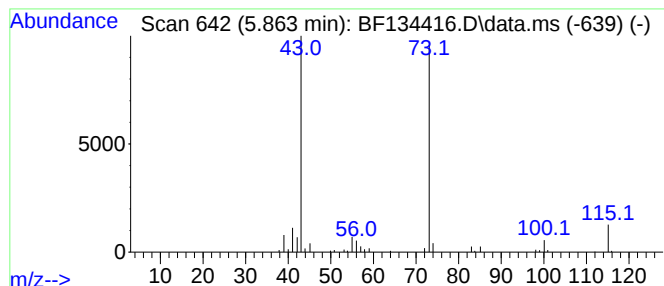
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.863	3.05 ng	68658	1,4-Dichlorobenzene-d4		6.840	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-		130	C7H14O2	000107-70-0	83
2	N-.alpha.-Acetylglycinamide		116	C4H8N2O2	002620-63-5	38
3	1,3-Dioxolane, 2-(1-methylethyl)-		116	C6H12O2	000822-83-3	27
4	3-Hexanol, acetate		144	C8H16O2	040780-64-1	25
5	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	14



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Instrument :
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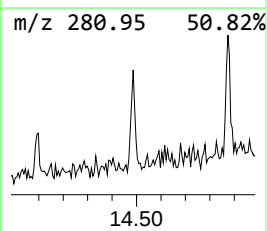
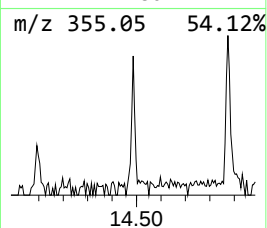
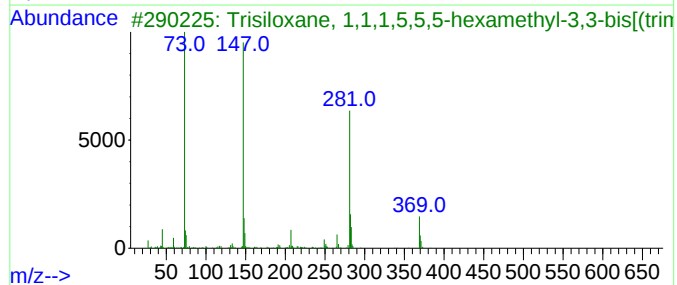
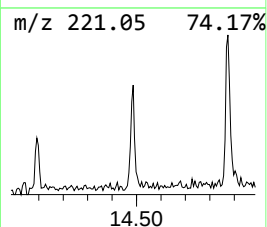
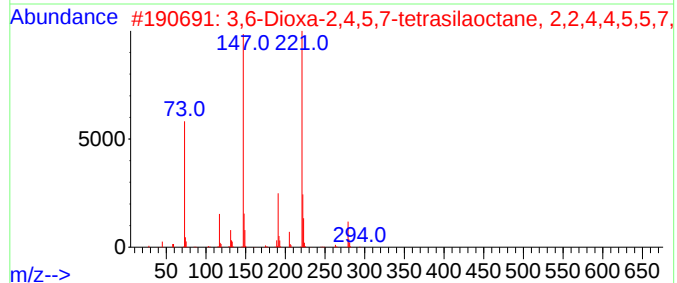
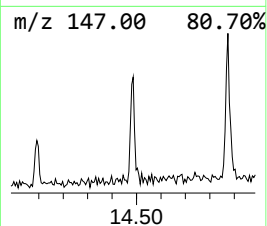
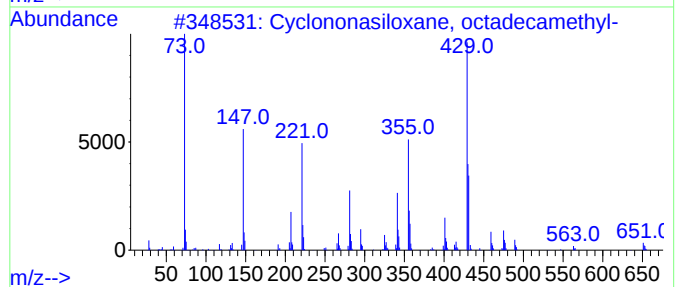
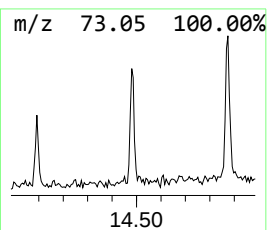
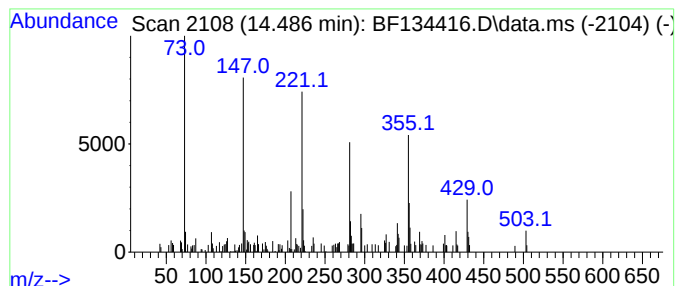
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Cyclononasiloxane, octadeca... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	2.37 ng	72845	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	64
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3			Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	25
4			3,4-Dihydroxyphenylglycol, 4TMS ...	458	C20H42O4Si4	056114-62-6	25
5			N-[4-(Aminosulfonyl)phenyl]propa...	444	C18H36N2O3SSi3	1000500-82-8	22



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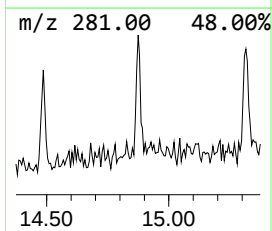
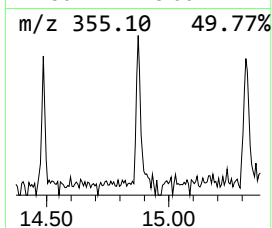
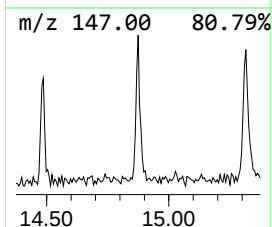
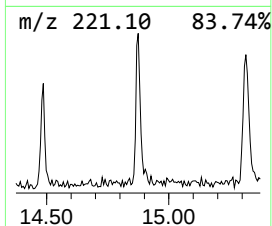
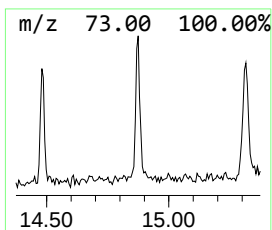
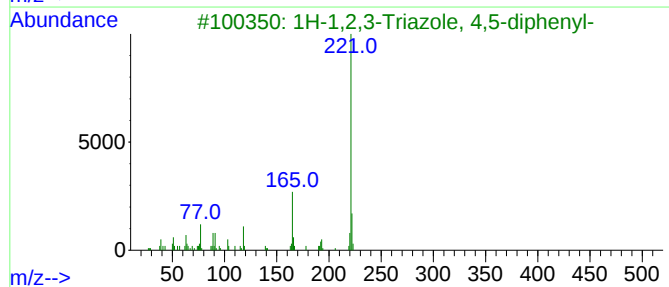
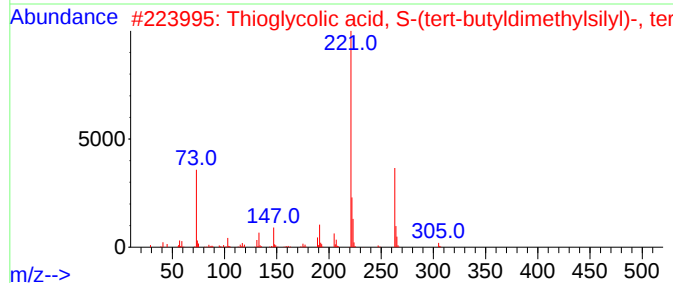
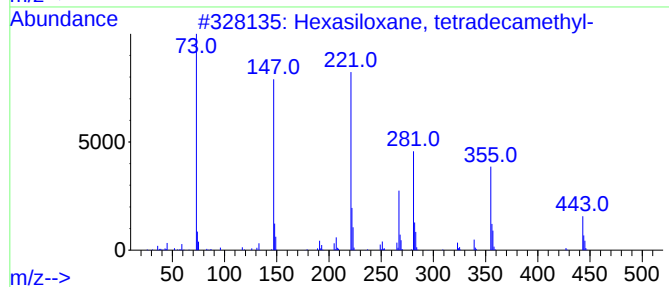
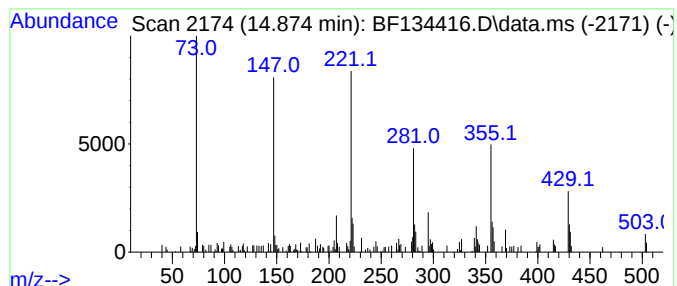
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Hexasiloxane, tetradecamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.874	2.32 ng	71633	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	72
2			Thioglycolic acid, S-(tert-butyl...	320	C14H32O2SSi2	082112-29-6	14
3			1H-1,2,3-Triazole, 4,5-diphenyl-	221	C14H11N3	005533-73-3	11
4			1,2-Dibenzoyl-3-phenylcyclopropane	326	C23H18O2	029128-64-1	11
5			1,3-Cyclohexanedione, 2-[2-[4-(4...	401	C22H28FN3O3	339310-26-8	11



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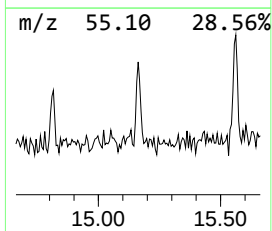
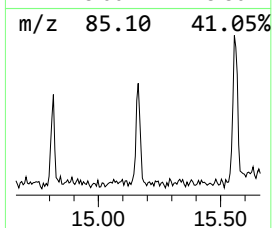
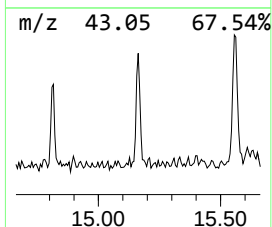
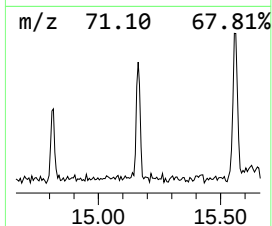
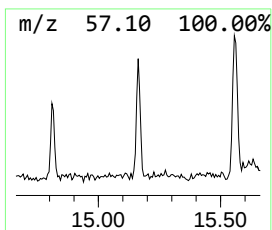
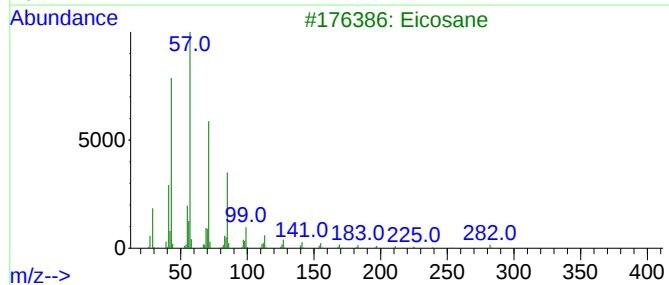
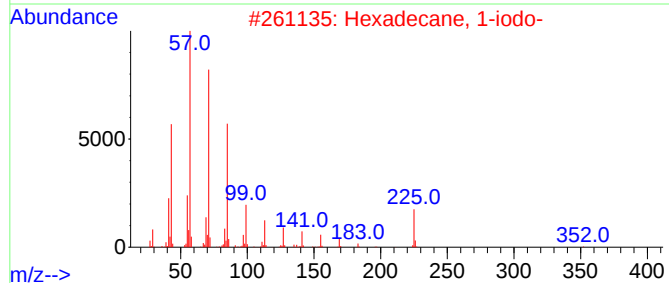
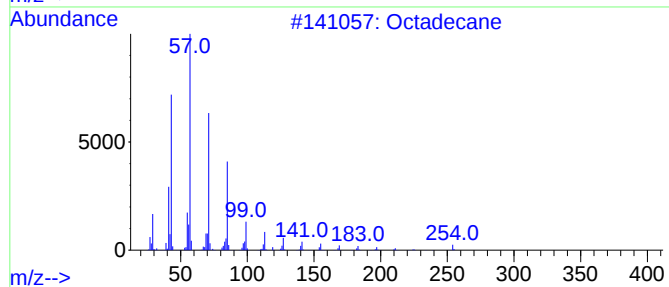
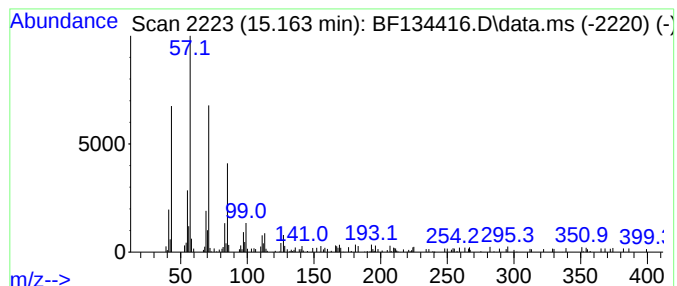
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.163	2.27 ng	70128	Perylene-d12	15.545

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	95
2		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	91
3		Eicosane	282	C20H42	000112-95-8	91
4		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87
5		Octacosane	394	C28H58	000630-02-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
Data File : BF134416.D
Acq On : 22 Jul 2023 11:46
Operator : CG\JU
Sample : PB154316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154316BL

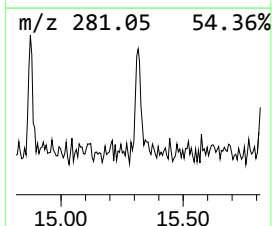
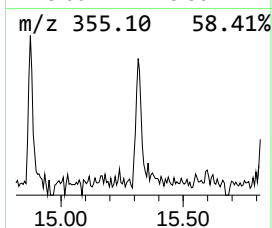
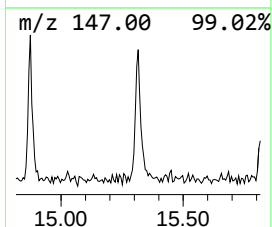
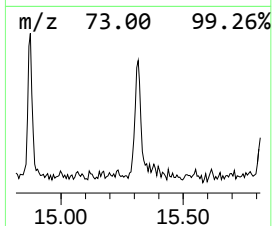
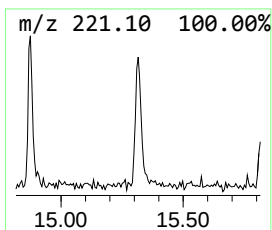
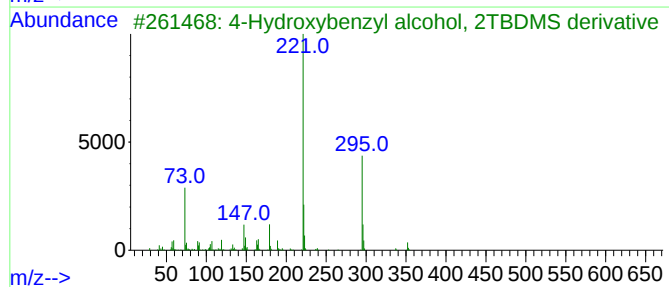
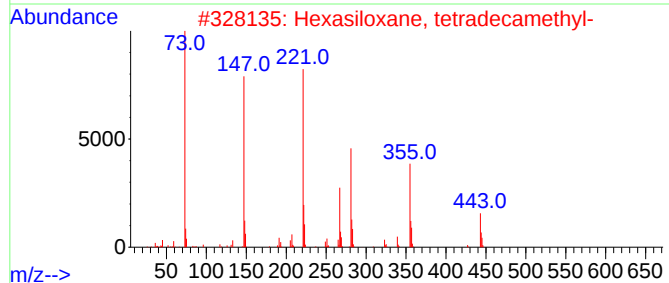
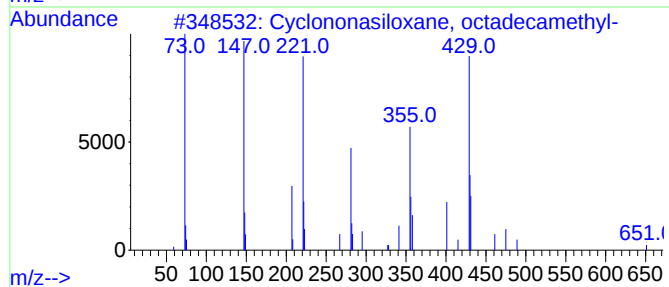
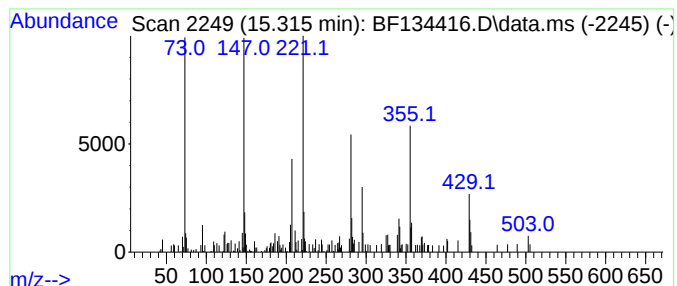
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.315 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.315	2.18 ng	67183	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			Hexasiloxane, tetradecamethyl-	458	C14H42O5Si6	000107-52-8	53
3			4-Hydroxybenzyl alcohol, 2TBDMS ...	352	C19H36O2Si2	1000364-43-9	25
4			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22
5			Heptasiloxane, hexadecamethyl-	532	C16H48O6Si7	000541-01-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
Data File : BF134416.D
Acq On : 22 Jul 2023 11:46
Operator : CG\JU
Sample : PB154316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154316BL

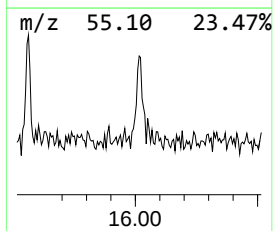
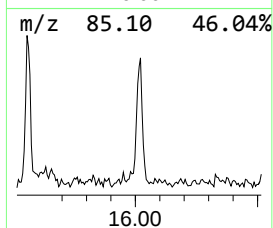
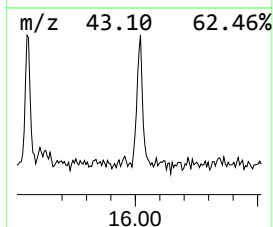
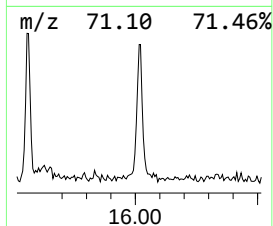
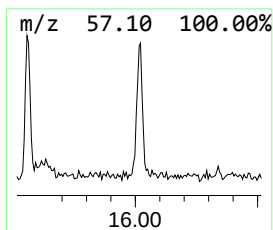
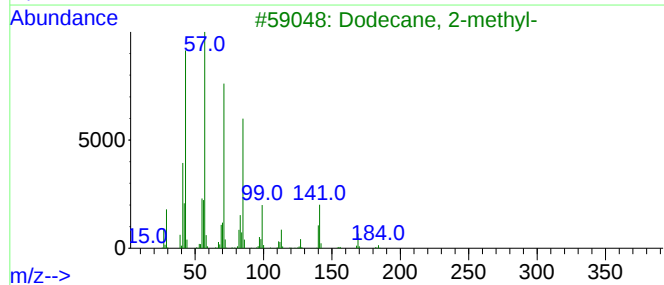
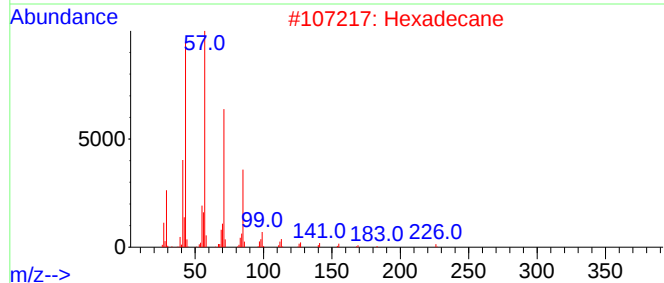
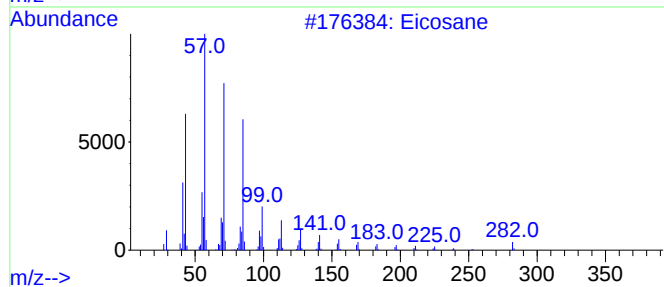
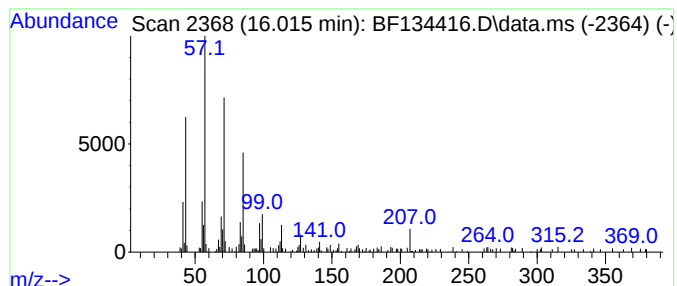
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	3.91 ng	120668	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Hexadecane	226	C16H34	000544-76-3	89
3			Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
4			Heneicosane	296	C21H44	000629-94-7	87
5			Tetratetracontane	619	C44H90	007098-22-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
Data File : BF134416.D
Acq On : 22 Jul 2023 11:46
Operator : CG\JU
Sample : PB154316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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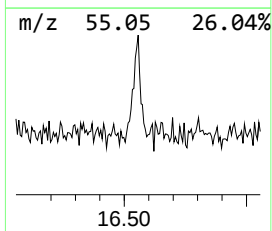
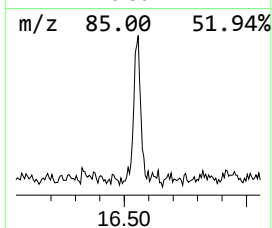
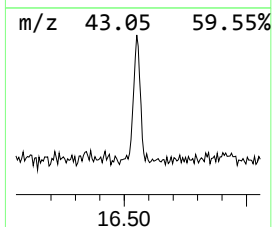
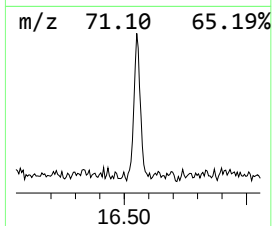
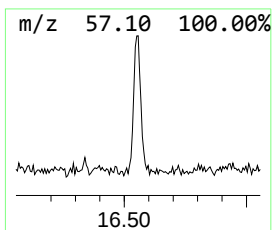
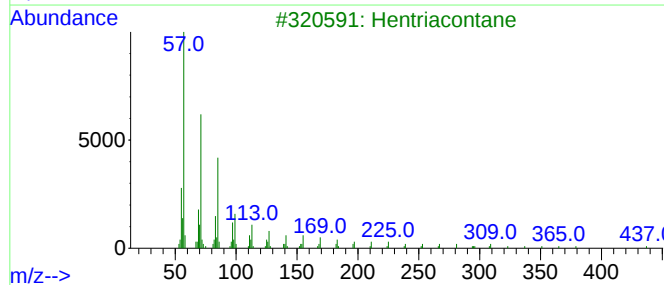
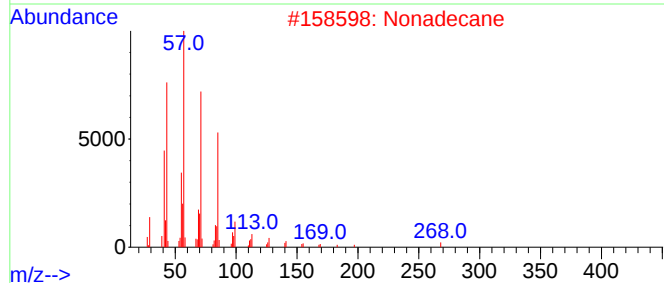
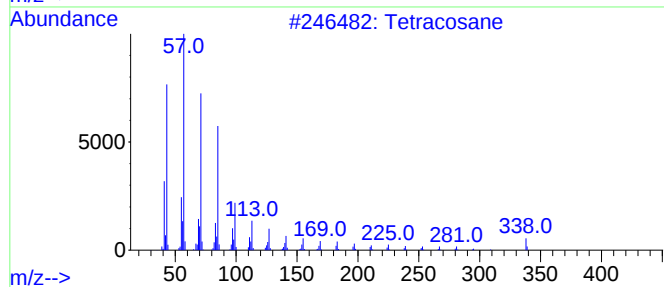
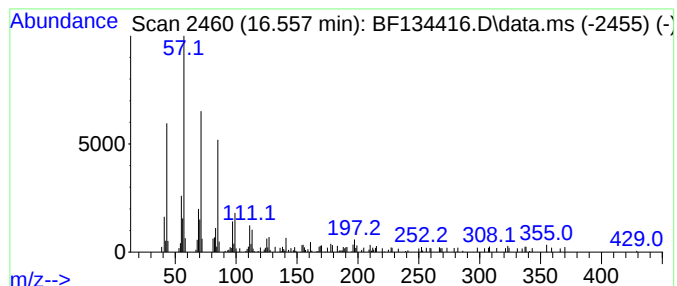
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.557	3.28 ng	101242	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	91
2			Nonadecane	268	C19H40	000629-92-5	89
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	87
5			11-Methyltricosane	338	C24H50	027538-41-6	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
Data File : BF134416.D
Acq On : 22 Jul 2023 11:46
Operator : CG\JU
Sample : PB154316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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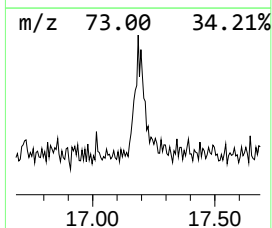
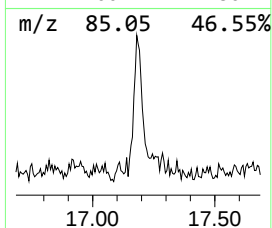
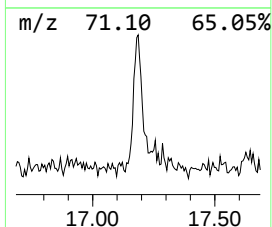
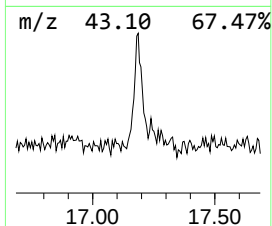
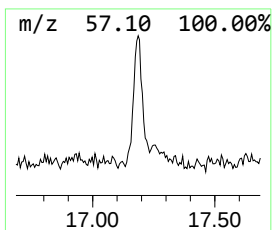
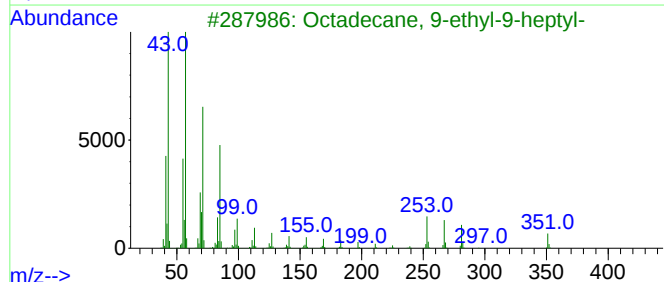
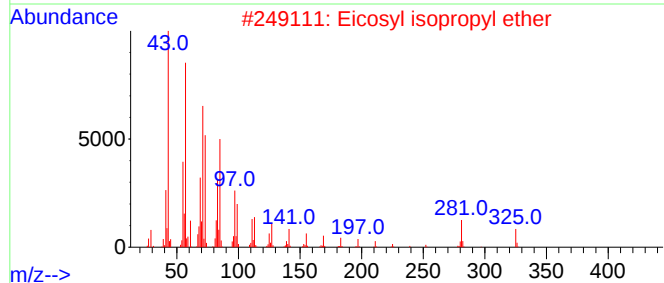
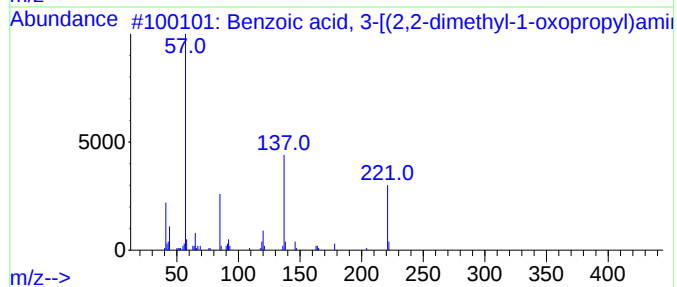
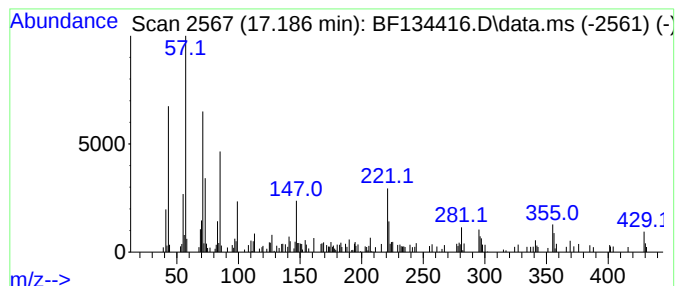
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown17.186 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.186	4.12 ng	127340	Perylene-d12	15.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 3-[(2,2-dimethyl-1...	221	C12H15NO3	056619-96-6	14
2			Eicosyl isopropyl ether	340	C23H48O	1000406-34-3	12
3			Octadecane, 9-ethyl-9-heptyl-	380	C27H56	055282-27-4	12
4			6,6-Diethylhooctadecane	310	C22H46	1000360-41-8	12
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072223\
Data File : BF134416.D
Acq On : 22 Jul 2023 11:46
Operator : CG\JU
Sample : PB154316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB154316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.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-...	5.104	89.2	ng	2011840	1	6.840	450861	20.0
2-Pentanone, 4-...	5.863	3.0	ng	68658	1	6.840	450861	20.0
Cyclononasiloxa...	14.486	2.4	ng	72845	5	14.039	614525	20.0
Hexasiloxane, t...	14.874	2.3	ng	71633	6	15.545	617701	20.0
Octadecane	15.163	2.3	ng	70128	6	15.545	617701	20.0
unknown15.315	15.315	2.2	ng	67183	6	15.545	617701	20.0
Eicosane	16.015	3.9	ng	120668	6	15.545	617701	20.0
Tetracosane	16.557	3.3	ng	101242	6	15.545	617701	20.0
unknown17.186	17.186	4.1	ng	127340	6	15.545	617701	20.0