

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
 Data File : BF138320.D
 Acq On : 24 Jun 2024 20:12
 Operator : CG\JU
 Sample : P3009-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-204

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-BF061224.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	21	rBV	2536951	3149297	80.47%	8.874%
2	5.075	503	508	510	rBV	36003	45105	1.15%	0.127%
3	5.104	510	513	522	rVB	201635	234734	6.00%	0.661%
4	5.510	577	582	585	rBV	3798439	3413202	87.21%	9.617%
5	6.516	748	753	756	rBV	3520864	3252352	83.10%	9.164%
6	6.886	812	816	819	rBV	1442292	1115164	28.49%	3.142%
7	7.445	907	911	914	rBV	2396310	2044284	52.23%	5.760%
8	8.169	1030	1034	1037	rBV	1610201	1327354	33.92%	3.740%
9	8.475	1083	1086	1095	rBV	106839	103477	2.64%	0.292%
10	9.239	1212	1216	1220	rBV	4347487	3789268	96.82%	10.677%
11	9.922	1328	1332	1335	rBV	1764539	1308249	33.43%	3.686%
12	10.016	1343	1348	1353	rBV	68436	88411	2.26%	0.249%
13	10.710	1462	1466	1469	rBV	2669860	2121367	54.20%	5.977%
14	11.410	1581	1585	1587	rBV	1562413	1317338	33.66%	3.712%
15	11.427	1587	1588	1592	rVB	190358	155167	3.96%	0.437%
16	11.510	1599	1602	1606	rBV2	44222	45482	1.16%	0.128%
17	11.616	1617	1620	1623	rBV	136829	137281	3.51%	0.387%
18	11.857	1658	1661	1665	rBV2	52841	79906	2.04%	0.225%
19	11.933	1671	1674	1681	rBV2	638687	577728	14.76%	1.628%
20	12.227	1722	1724	1727	rVB	52643	43729	1.12%	0.123%
21	12.621	1787	1791	1796	rBV	729375	707430	18.08%	1.993%
22	12.716	1804	1807	1811	rBV	198158	195745	5.00%	0.552%
23	12.851	1824	1830	1835	rVB	553520	609997	15.59%	1.719%
24	12.992	1850	1854	1858	rVB	4348799	3913666	100.00%	11.028%
25	13.680	1969	1971	1974	rVB	83702	74488	1.90%	0.210%
26	13.892	2004	2007	2012	rBV	381656	466050	11.91%	1.313%
27	14.045	2028	2033	2036	rBV2	1266424	1477254	37.75%	4.162%
28	14.074	2036	2038	2043	rVB	349543	309378	7.91%	0.872%
29	14.674	2137	2140	2144	rBV	614309	677636	17.31%	1.909%
30	14.904	2176	2179	2186	rVB2	405700	473167	12.09%	1.333%
31	14.974	2188	2191	2195	rVB	386476	376260	9.61%	1.060%
32	15.092	2208	2211	2219	rVB	282261	603743	15.43%	1.701%
33	15.198	2226	2229	2236	rVB2	330320	449514	11.49%	1.267%
34	15.527	2281	2285	2289	rBV	689576	806472	20.61%	2.272%

Sum of corrected areas: 35489695

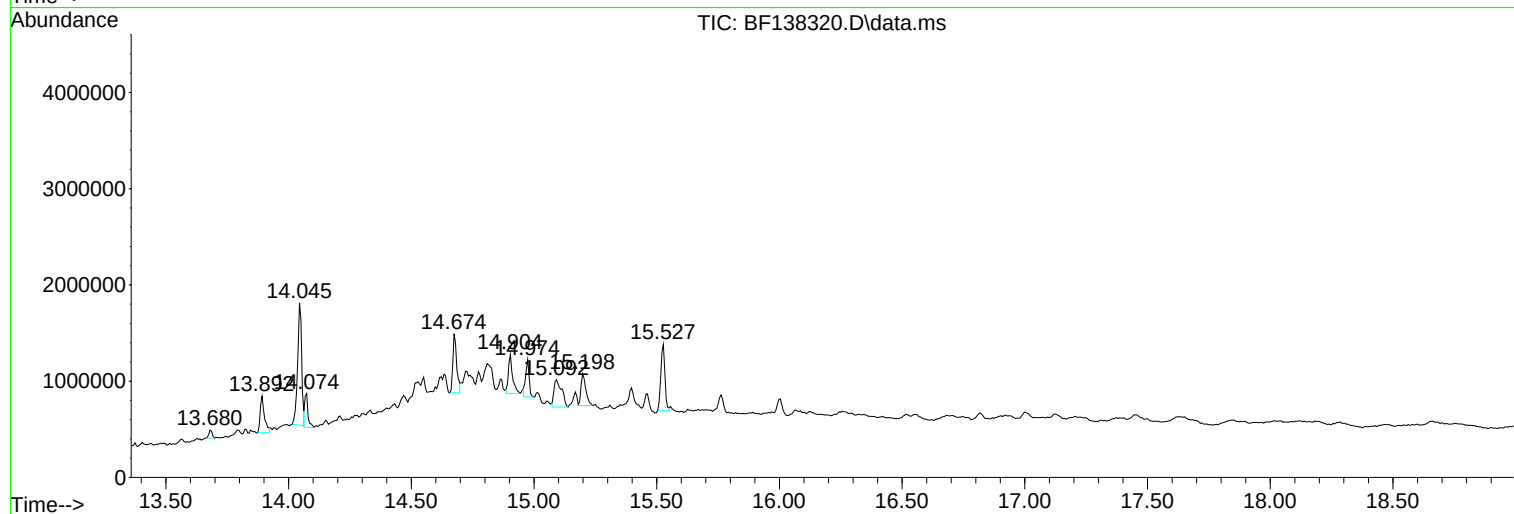
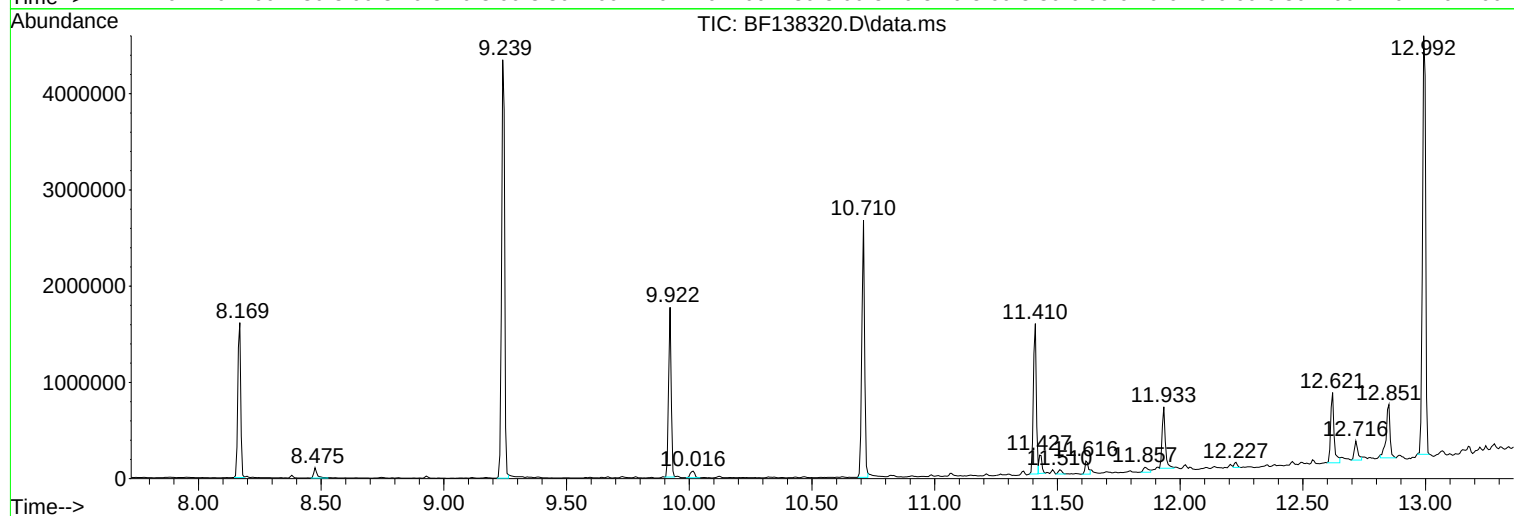
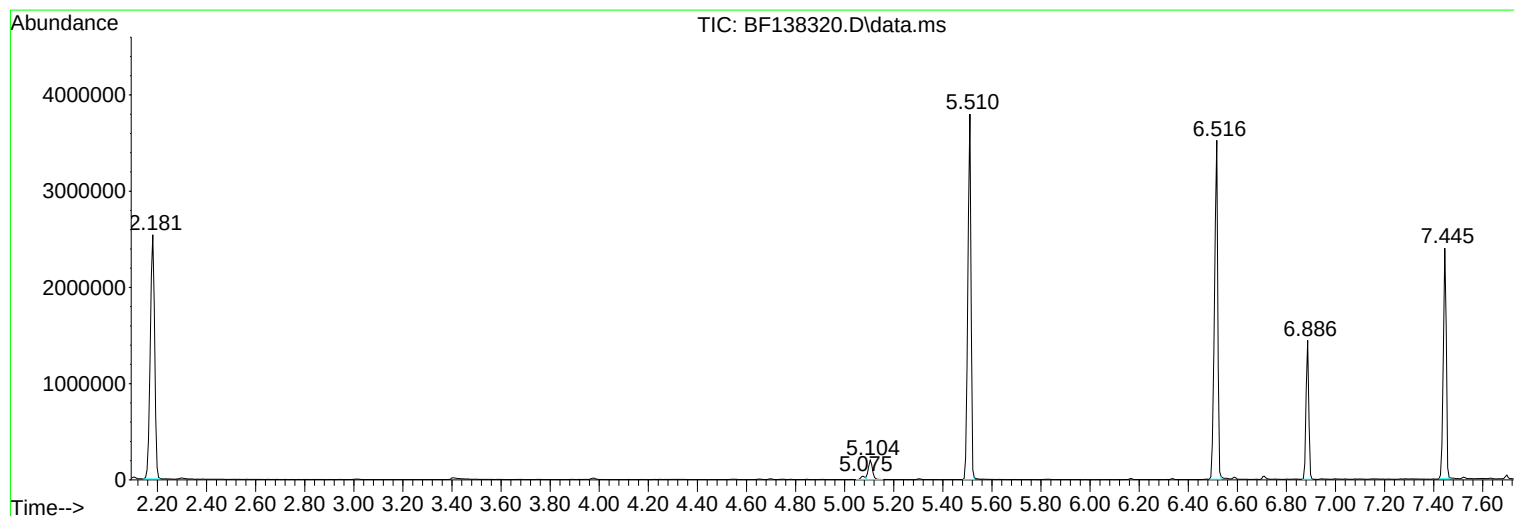
Instrument :
BNA_F
ClientSampleId :
VNJ-204

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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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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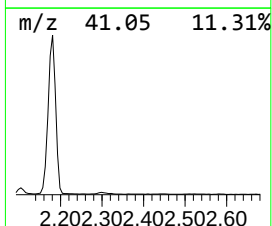
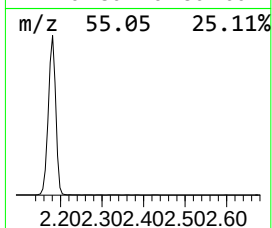
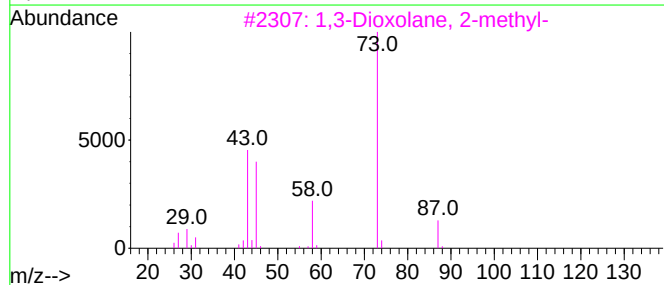
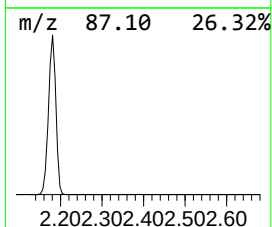
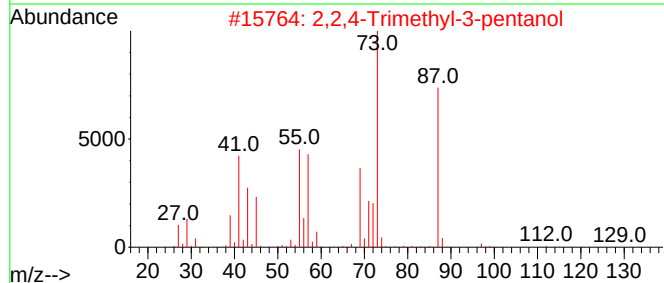
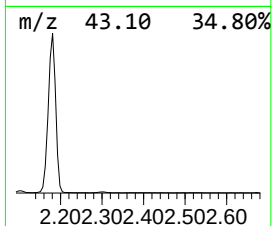
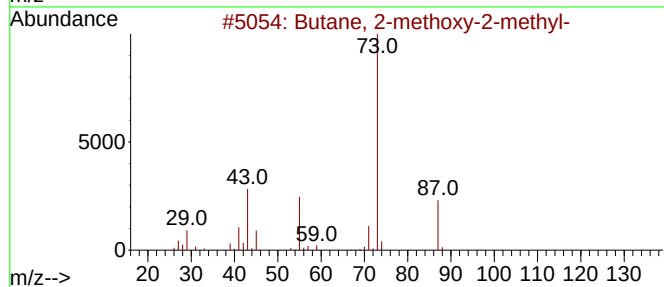
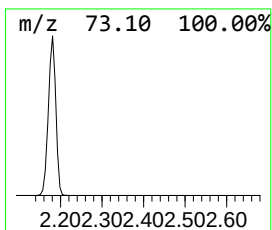
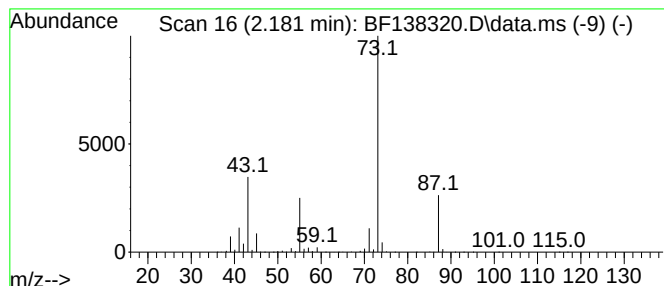
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	56.48 ng	3149300	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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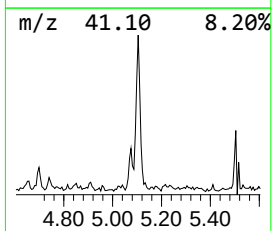
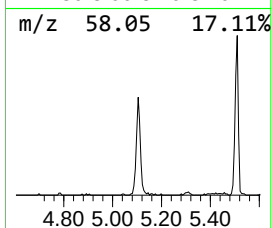
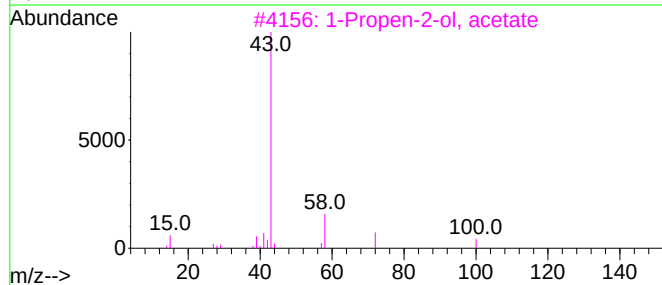
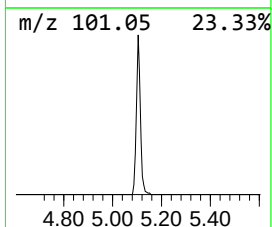
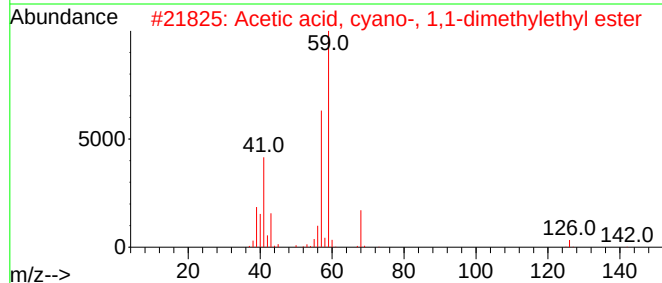
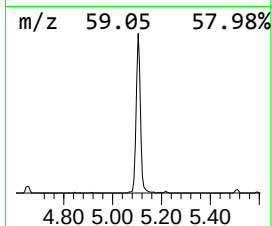
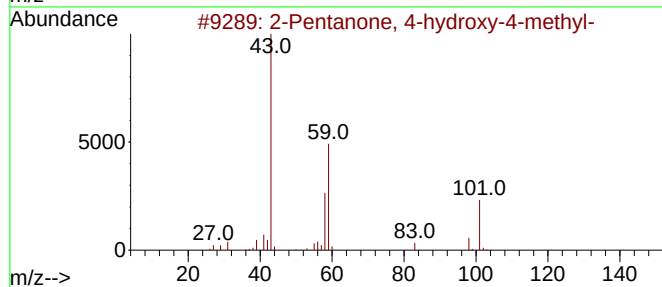
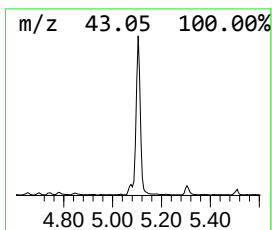
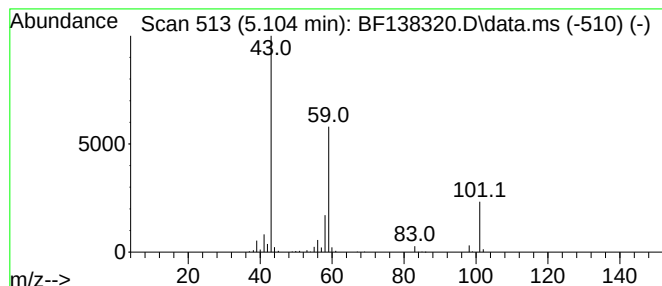
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.104	4.21 ng	234734	1,4-Dichlorobenzene-d4	6.886

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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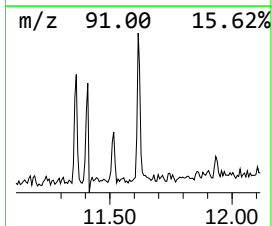
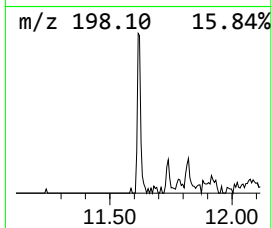
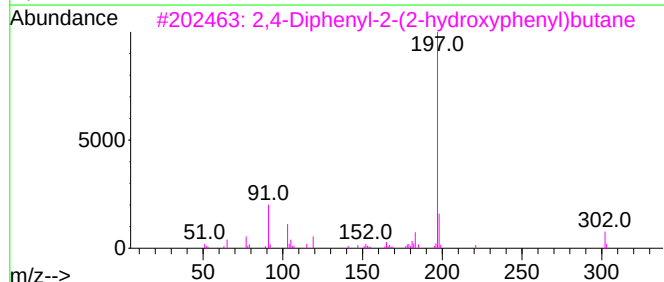
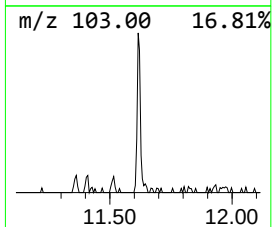
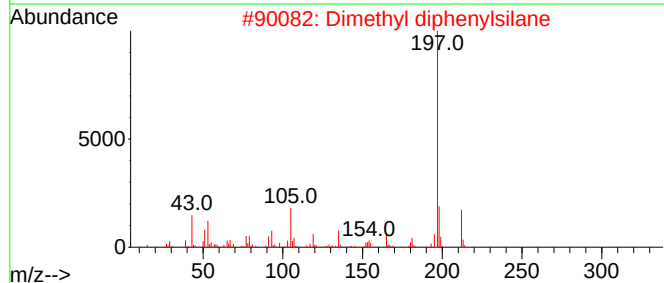
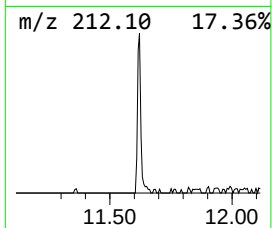
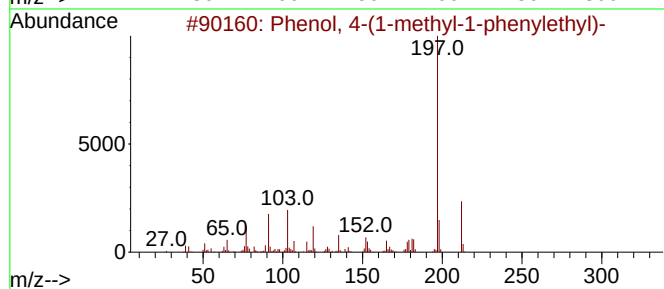
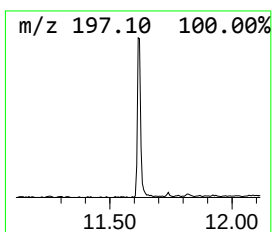
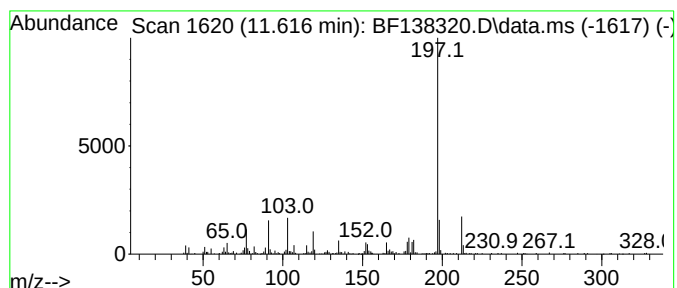
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenol, 4-(1-methyl-1-pheny... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.616	2.08 ng	137281	Phenanthrene-d10	11.410	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1-methyl-1-phenylethyl)-	212	C15H16O	000599-64-4	99
2	Dimethyl diphenylsilane	212	C14H16Si	000778-24-5	83
3	2,4-Diphenyl-2-(2-hydroxyphenyl)...	302	C22H22O	1000280-74-0	72
4	2,3-Dimethyl-4-biphenylamine	197	C14H15N	022750-87-4	62
5	Benzenemethanol, 2,3,4,5,6-penta...	212	C8H5F5O	000830-50-2	59



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VNJ-204

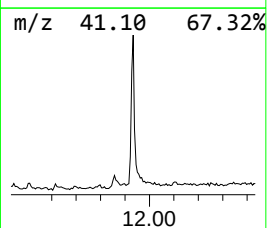
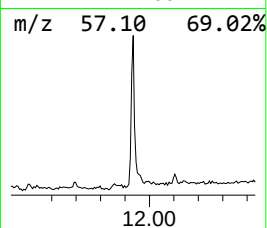
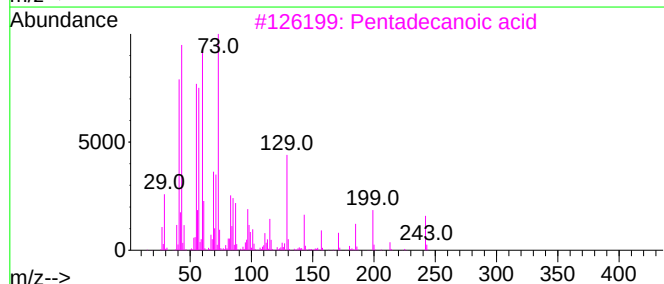
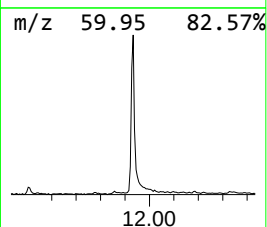
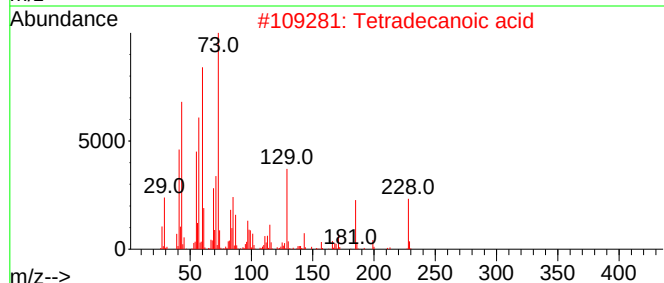
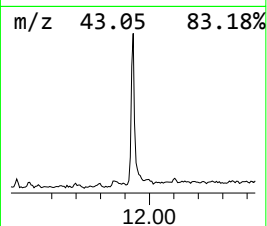
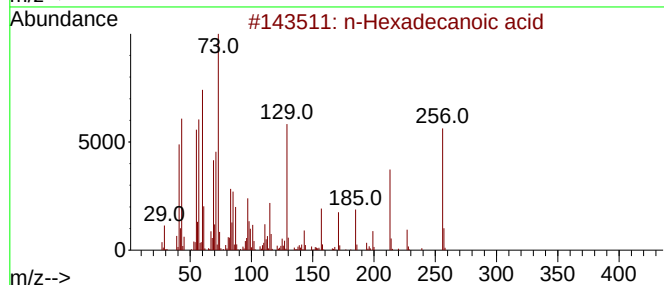
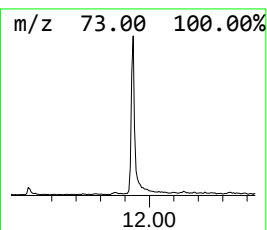
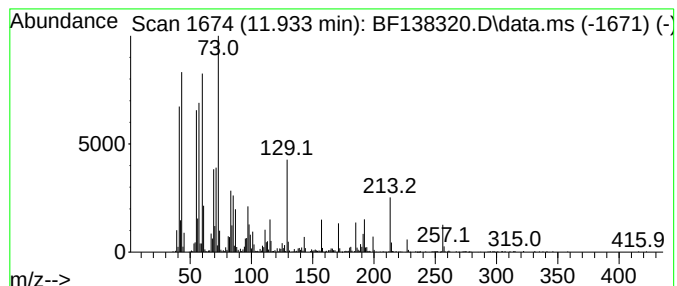
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	8.77 ng	577728	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Octadecanoic acid	284	C18H36O2	000057-11-4	93
5			Undecanoic acid	186	C11H22O2	000112-37-8	87



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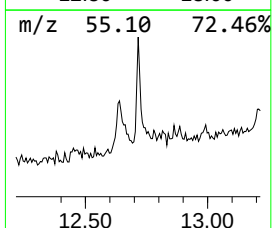
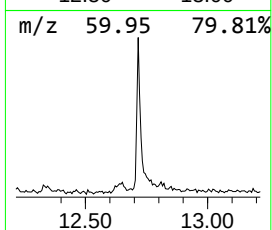
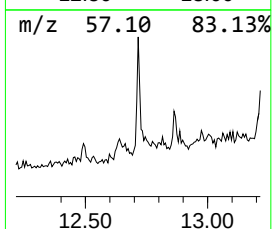
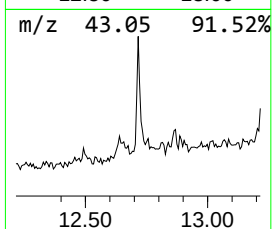
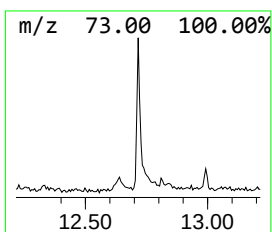
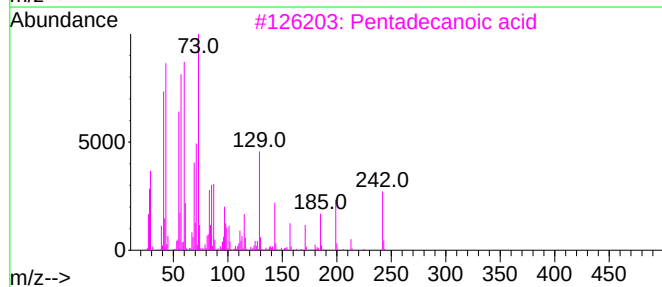
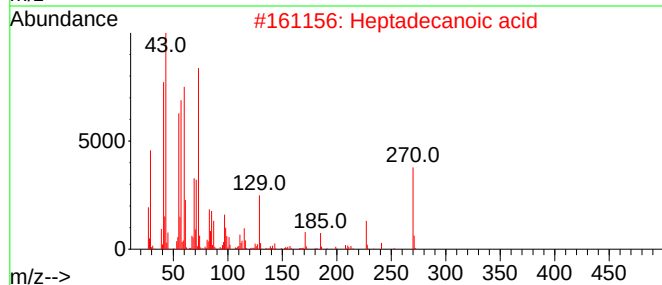
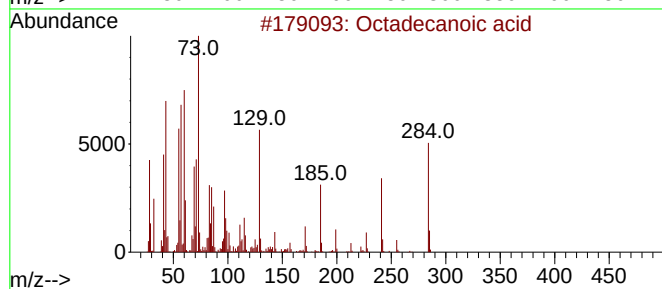
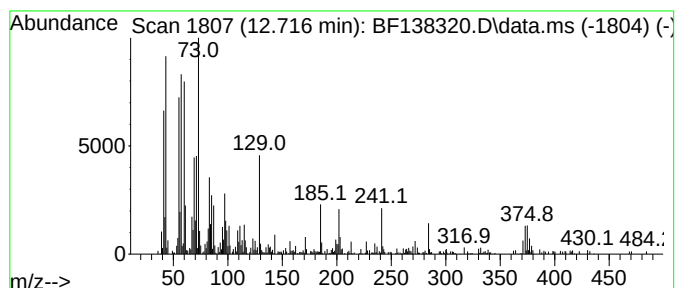
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.97 ng	195745	Phenanthrene-d10	11.410

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	78
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	70
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	60



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Misc :
ALS Vial : 21 Sample Multiplier: 1

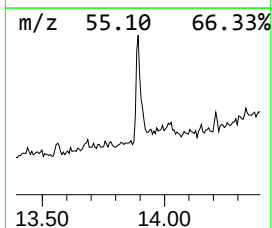
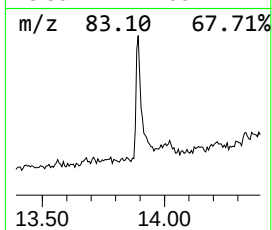
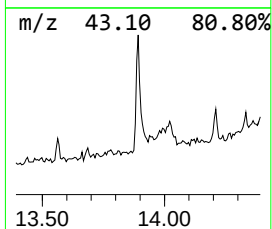
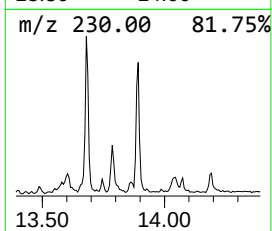
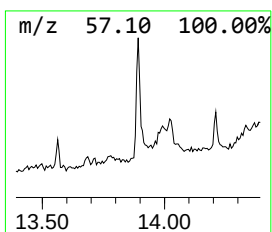
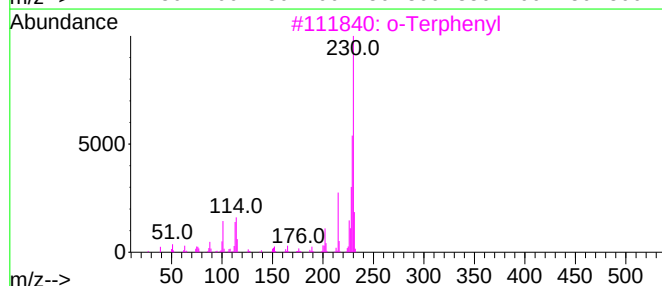
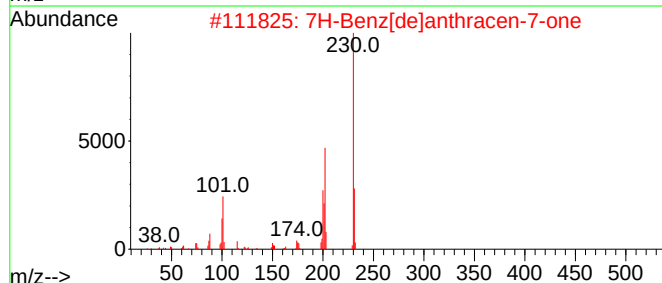
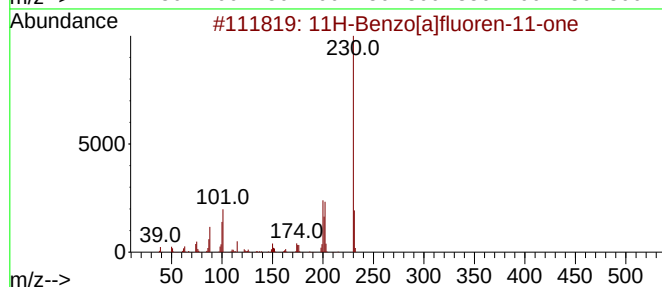
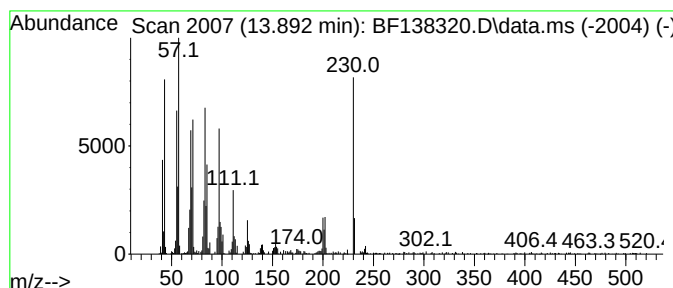
Instrument :
BNA_F
ClientSampleId :
VNJ-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.892	6.31 ng	466050	Chrysene-d12	14.045	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	59
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	25
3	o-Terphenyl	230	C18H14	000084-15-1	11
4	Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	11
5	Benzo(b)phenazine	230	C16H10N2	000257-97-6	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
Data File : BF138320.D
Acq On : 24 Jun 2024 20:12
Operator : CG\JU
Sample : P3009-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

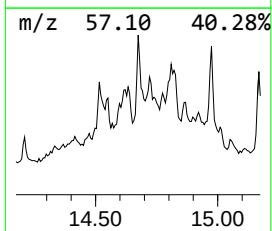
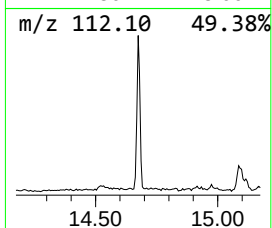
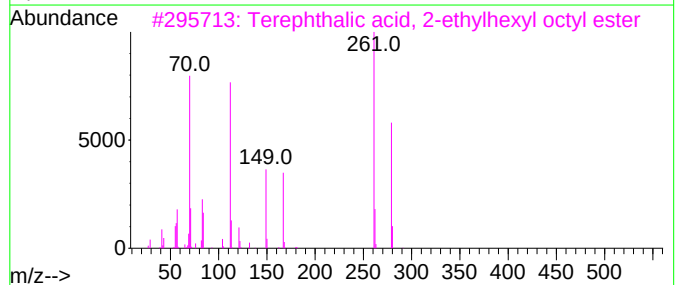
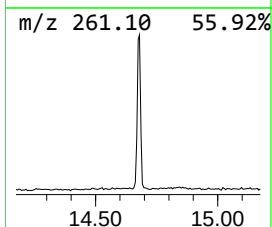
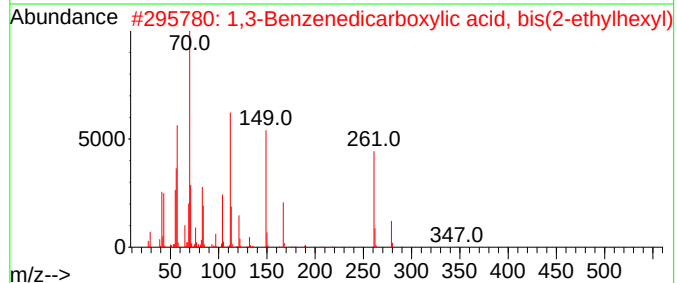
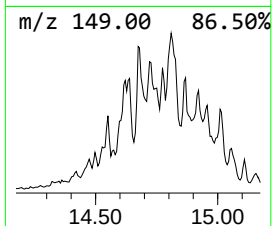
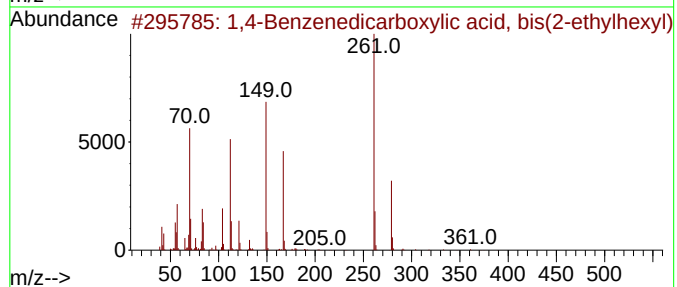
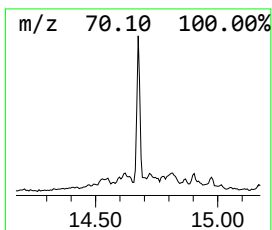
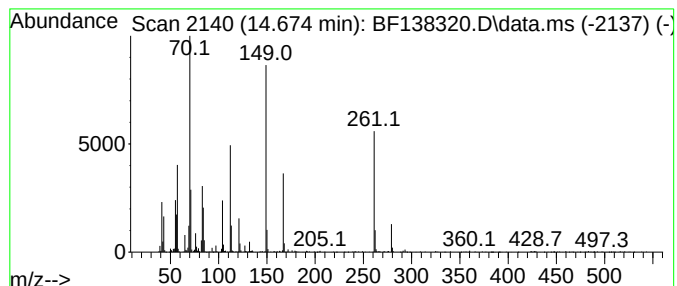
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ClientSampleId :
VNJ-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
14.674	9.17 ng	677636	Chrysene-d12			14.045
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...		390	C24H38O4	006422-86-2	76
2	1,3-Benzenedicarboxylic acid, bi...		390	C24H38O4	000137-89-3	64
3	Terephthalic acid, 2-ethylhexyl ...		390	C24H38O4	1000324-00-5	52
4	Isophthalic acid, 3-methylbut-2-...		348	C21H32O4	1000344-72-4	43
5	Terephthalic acid, monochloride,...		296	C16H21ClO3	1000324-22-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
Data File : BF138320.D
Acq On : 24 Jun 2024 20:12
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Sample : P3009-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VNJ-204

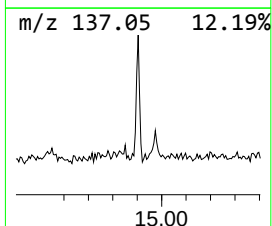
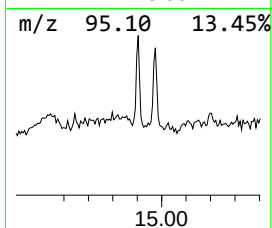
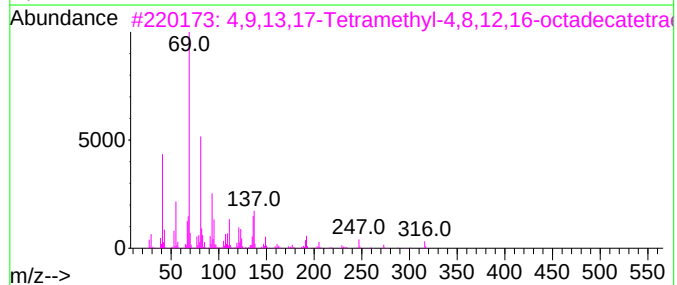
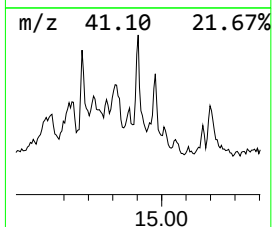
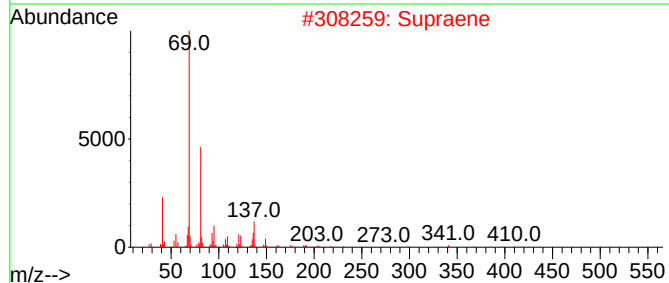
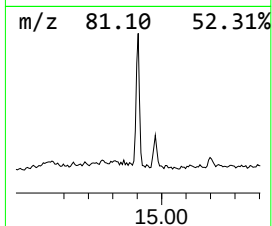
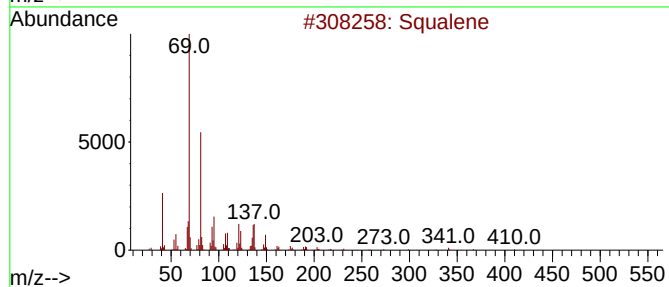
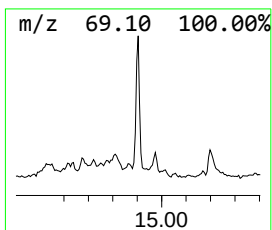
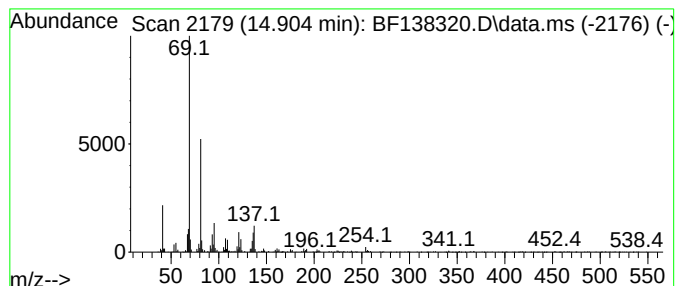
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.904	11.73 ng	473167	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	92
2			Supraene	410	C30H50	007683-64-9	87
3			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	72
5			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
Data File : BF138320.D
Acq On : 24 Jun 2024 20:12
Operator : CG\JU
Sample : P3009-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-204

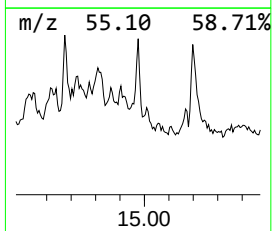
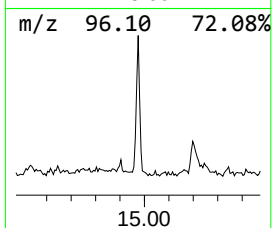
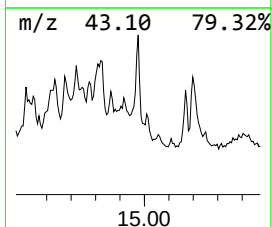
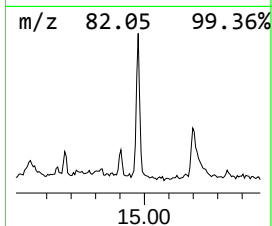
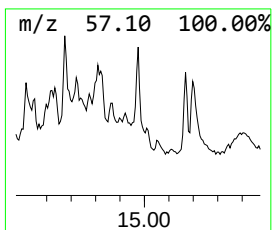
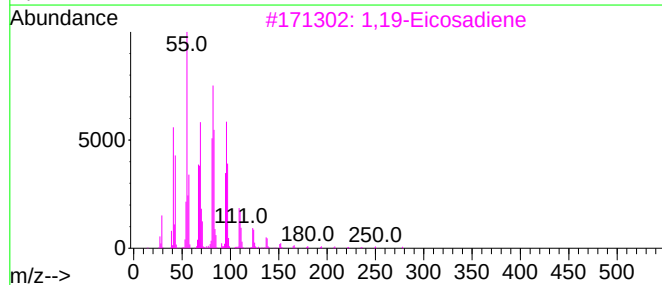
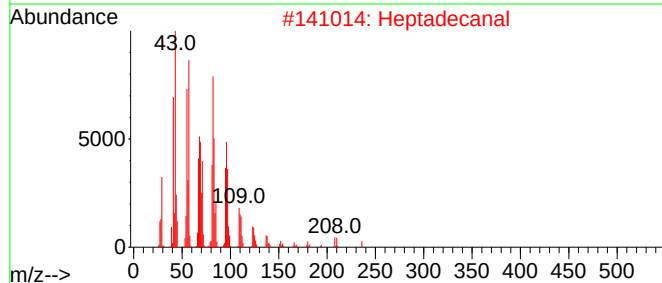
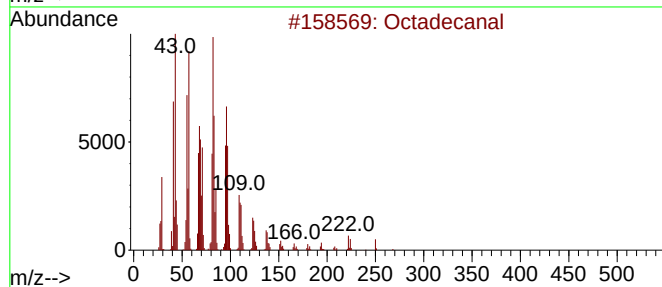
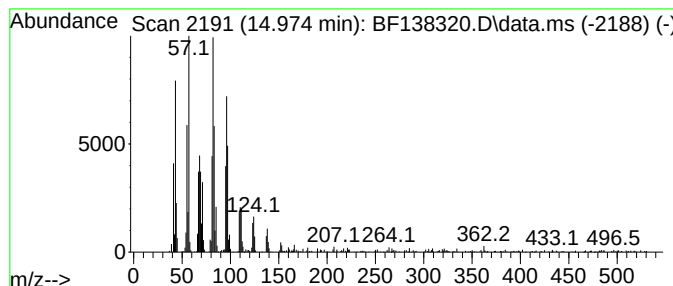
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.974	9.33 ng	376260	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	95
2			Heptadecanal	254	C17H34O	1000376-70-0	94
3			1,19-Eicosadiene	278	C20H38	014811-95-1	90
4			Hexacosanal	380	C26H52O	026627-85-0	87
5			9-Octadecen-1-ol, (E)-	268	C18H36O	000506-42-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
Data File : BF138320.D
Acq On : 24 Jun 2024 20:12
Operator : CG\JU
Sample : P3009-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-204

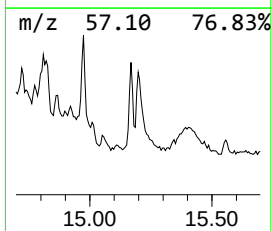
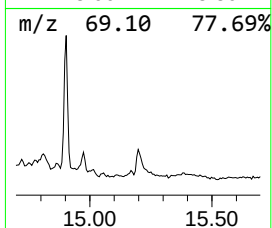
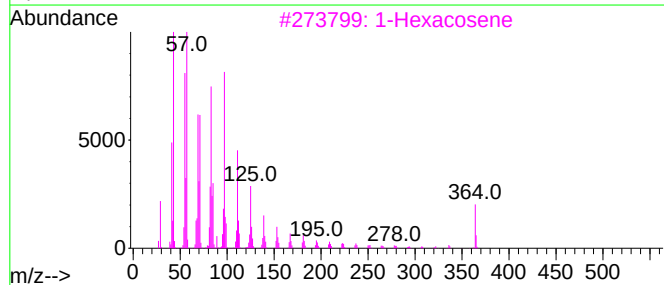
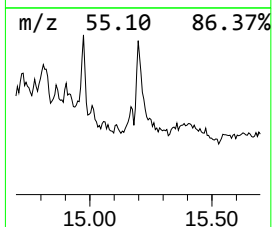
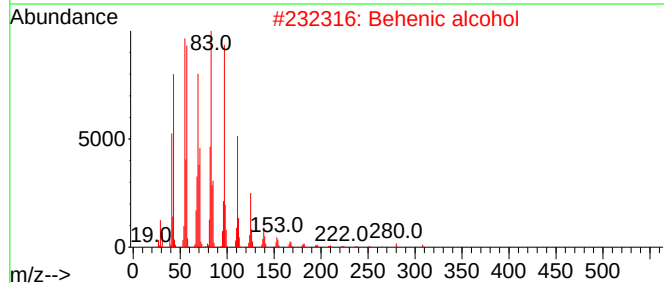
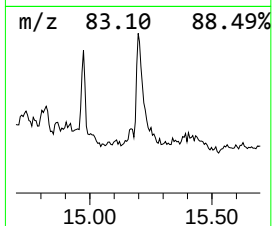
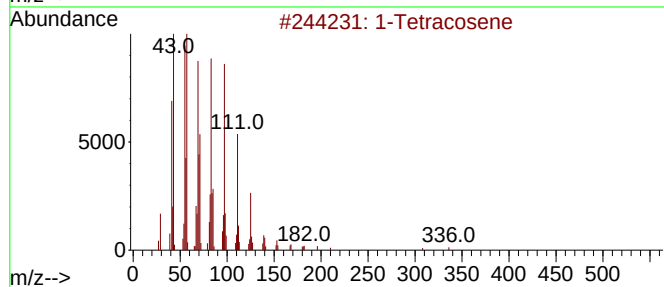
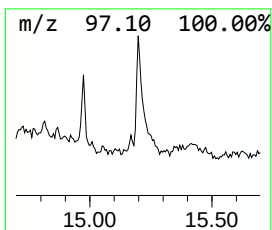
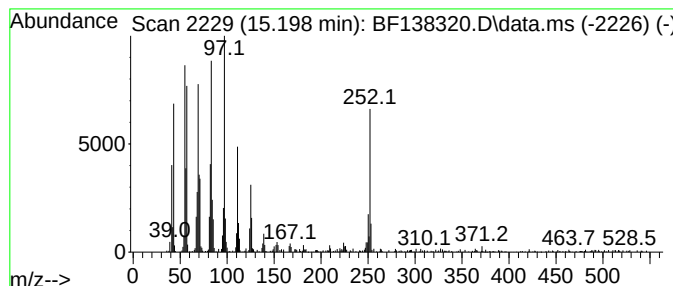
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Tetracosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.198	11.15 ng	449514	Perylene-d12	15.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Tetracosene	336	C24H48	010192-32-2	93
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		5-Octadecene, (E)-	252	C18H36	007206-21-5	87
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF062424\
Data File : BF138320.D
Acq On : 24 Jun 2024 20:12
Operator : CG\JU
Sample : P3009-01
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-204

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF061224.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
Butane, 2-metho...	2.181	56.5	ng	3149300	1	6.886	1115160	20.0
2-Pentanone, 4-...	5.104	4.2	ng	234734	1	6.886	1115160	20.0
Phenol, 4-(1-me...	11.616	2.1	ng	137281	4	11.410	1317340	20.0
n-Hexadecanoic ...	11.933	8.8	ng	577728	4	11.410	1317340	20.0
Octadecanoic acid	12.716	3.0	ng	195745	4	11.410	1317340	20.0
11H-Benzo[a]flu...	13.892	6.3	ng	466050	5	14.045	1477250	20.0
1,4-Benzenedica...	14.674	9.2	ng	677636	5	14.045	1477250	20.0
Squalene	14.904	11.7	ng	473167	6	15.527	806472	20.0
Octadecanal	14.974	9.3	ng	376260	6	15.527	806472	20.0
1-Tetracosene	15.198	11.2	ng	449514	6	15.527	806472	20.0