

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
 Data File : BF128522.D
 Acq On : 27 May 2022 21:29
 Operator : CG\JU
 Sample : N2921-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P013-SS002-0006-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128522.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.410	357	361	366	rBV2	125299	144646	2.32%	0.348%
2	4.851	433	436	445	rBV2	117628	156246	2.50%	0.376%
3	5.075	471	474	482	rVB	141423	176148	2.82%	0.423%
4	5.457	533	539	542	rBV	4830153	5180153	83.02%	12.454%
5	6.463	703	710	713	rBV	4622025	5298745	84.92%	12.739%
6	6.575	726	729	736	rVB	107576	89945	1.44%	0.216%
7	6.834	770	773	777	rBV	1484370	1319184	21.14%	3.171%
8	7.398	863	869	872	rBV	3441864	3680004	58.98%	8.847%
9	8.116	987	991	995	rBV	1854688	1738941	27.87%	4.181%
10	9.198	1169	1175	1178	rBV	6309646	6239419	100.00%	15.000%
11	9.875	1283	1290	1293	rBV	2241340	1909304	30.60%	4.590%
12	10.663	1418	1424	1427	rBV	3669079	3446595	55.24%	8.286%
13	11.363	1539	1543	1546	rBV	2071731	1803483	28.90%	4.336%
14	11.892	1629	1633	1637	rBV	244979	248500	3.98%	0.597%
15	12.674	1763	1766	1772	rBV	163474	188878	3.03%	0.454%
16	12.951	1808	1813	1817	rBV	4870787	5064662	81.17%	12.176%
17	13.892	1969	1973	1987	rVB2	126045	317560	5.09%	0.763%
18	13.998	1987	1991	1994	rBV	1325539	1210341	19.40%	2.910%
19	14.098	2002	2008	2018	rBV	967719	1242250	19.91%	2.987%
20	14.486	2070	2074	2077	rBV	134873	129974	2.08%	0.312%
21	15.133	2181	2184	2189	rVB	114452	132311	2.12%	0.318%
22	15.463	2235	2240	2245	rBV	822895	1034929	16.59%	2.488%
23	15.957	2320	2324	2330	rVB2	106264	150622	2.41%	0.362%
24	16.757	2456	2460	2467	rVB3	58965	106318	1.70%	0.256%
25	17.062	2507	2512	2519	rVB2	101969	206978	3.32%	0.498%
26	17.604	2595	2604	2617	rBV10	102205	378979	6.07%	0.911%

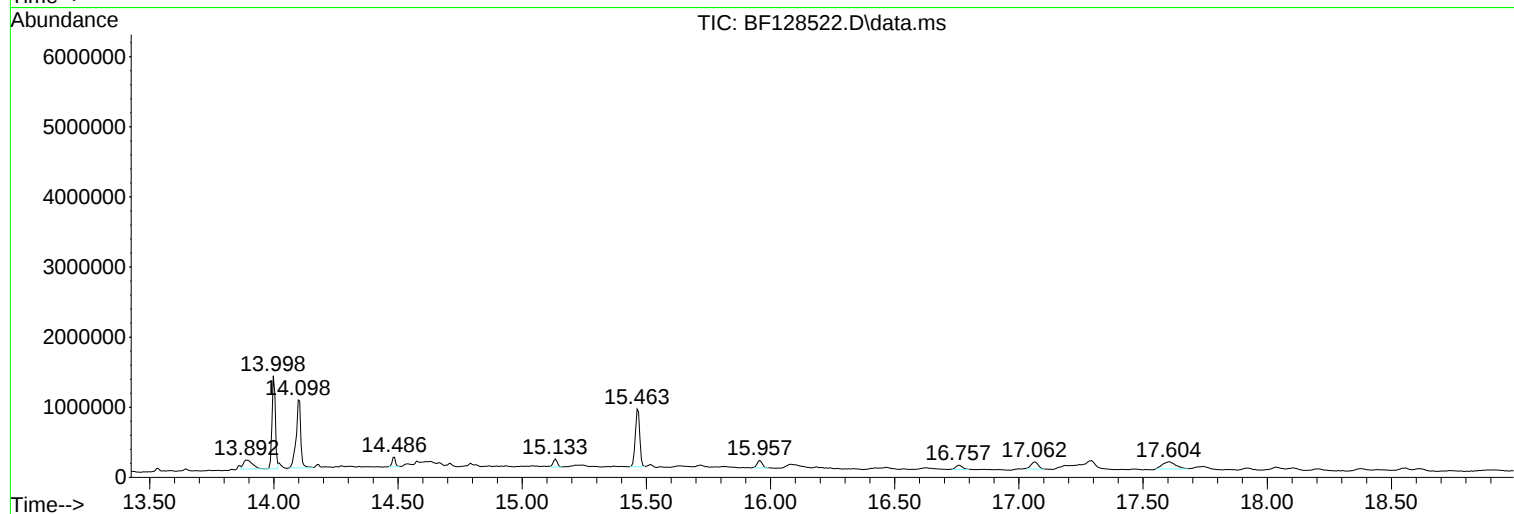
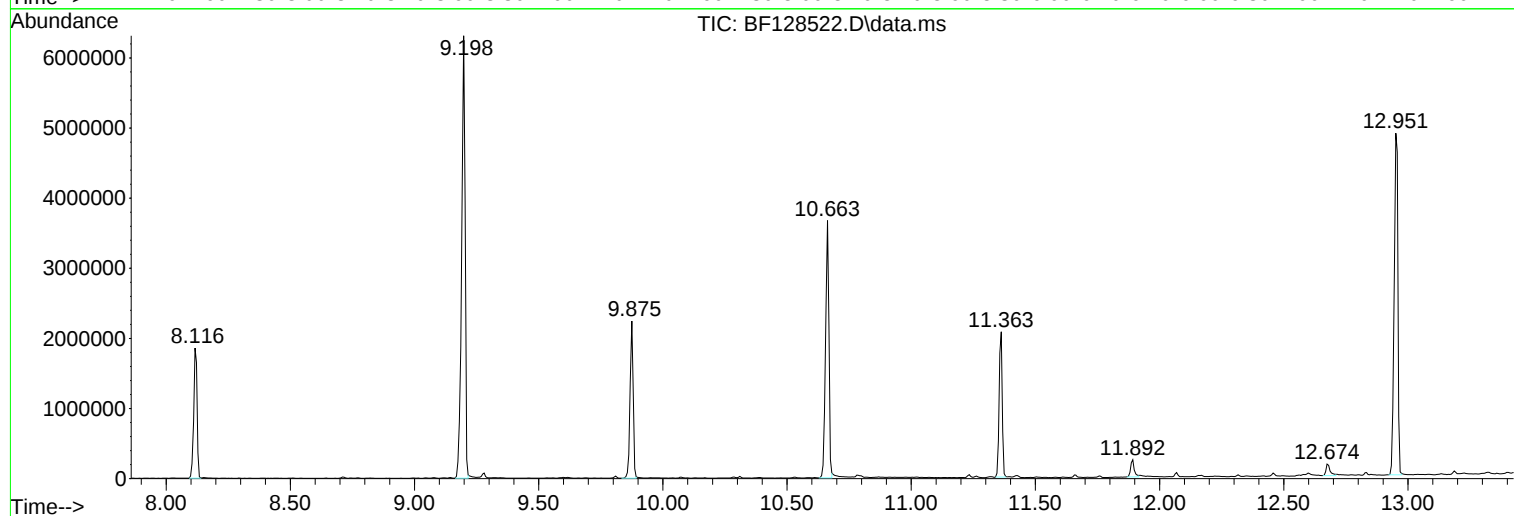
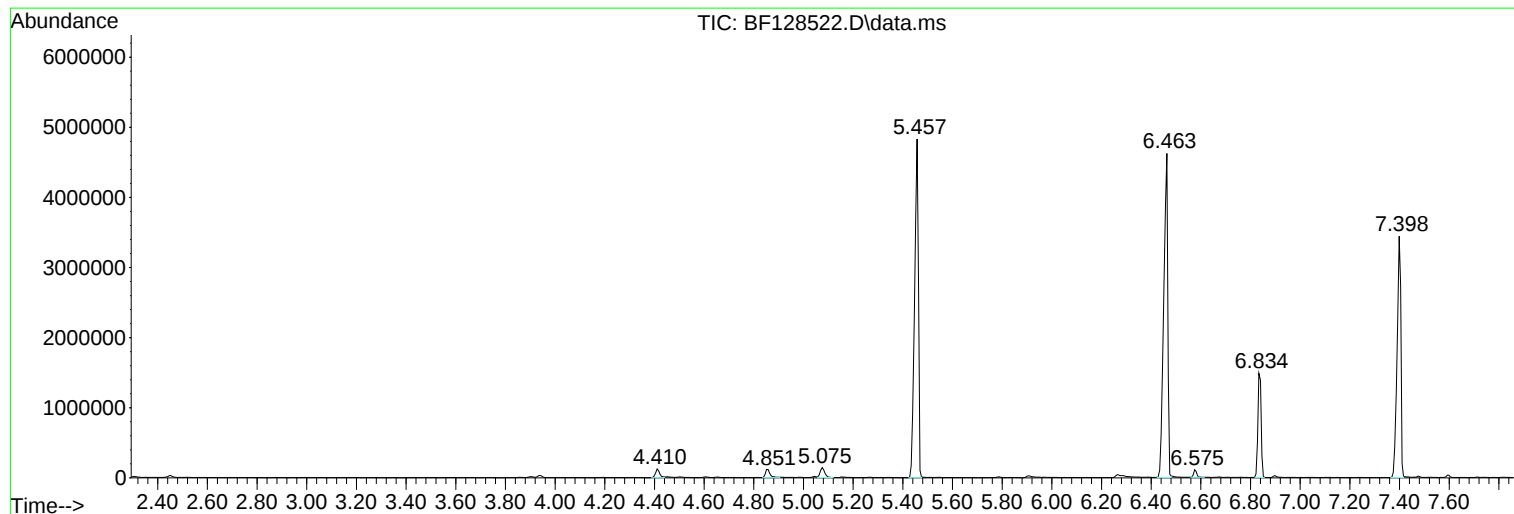
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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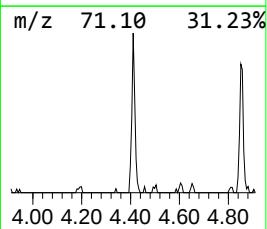
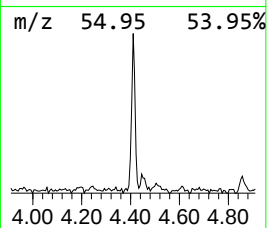
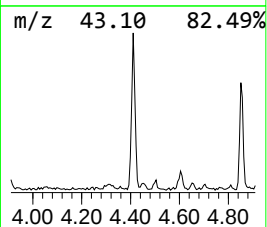
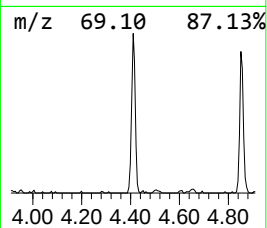
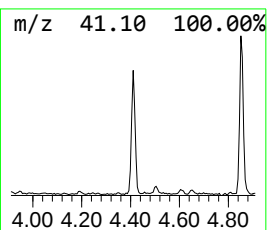
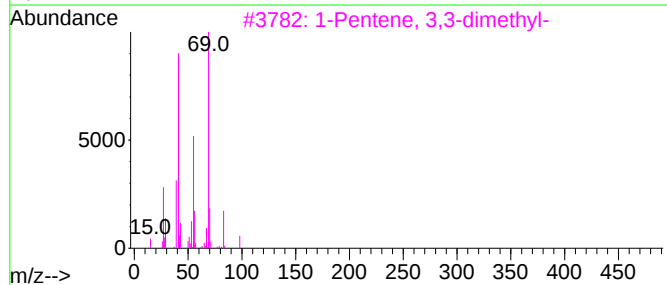
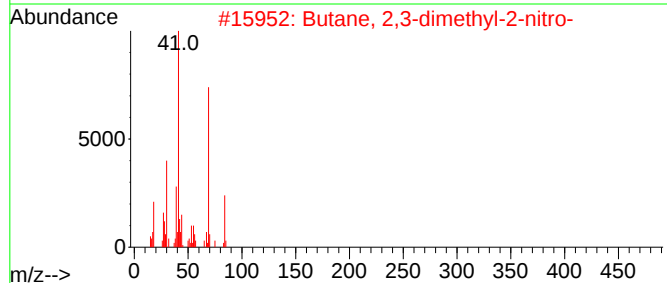
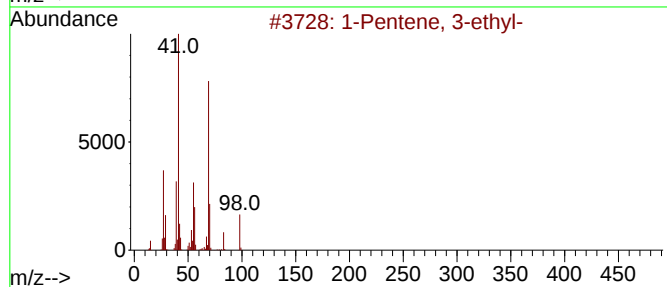
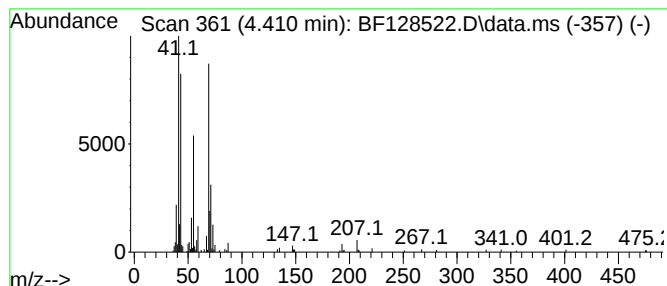
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Pentene, 3-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.410	2.19 ng	144646	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	50
2			Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	43
3			1-Pentene, 3,3-dimethyl-	98	C7H14	003404-73-7	40
4			1-Octene, 3,3-dimethyl-	140	C10H20	074511-51-6	40
5			2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	40



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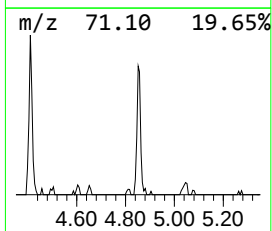
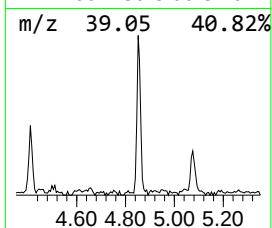
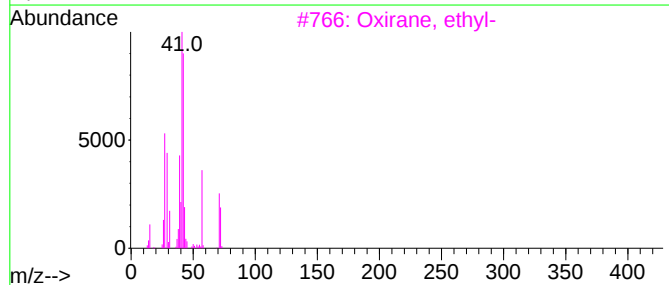
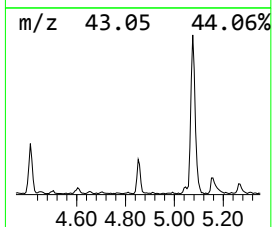
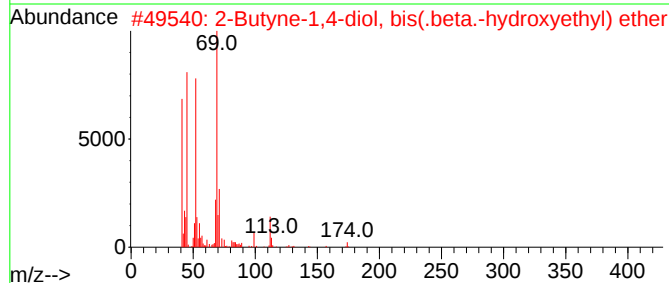
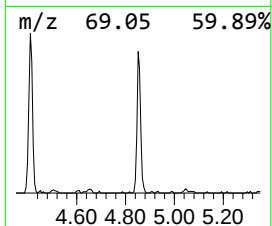
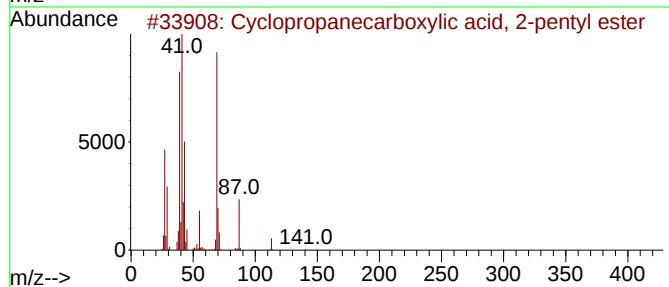
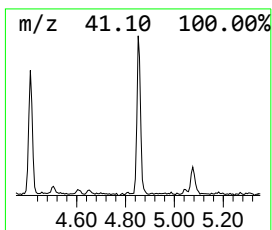
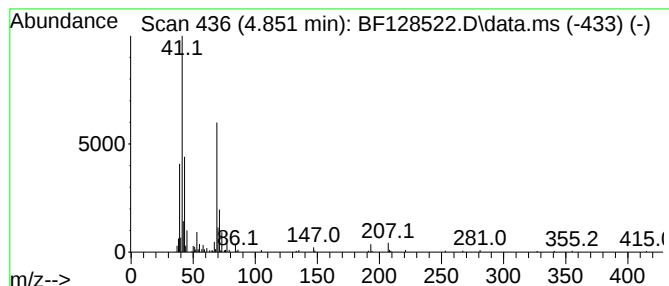
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.851 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.851	2.37 ng	156246	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, 2-p...	156	C9H16O2	1000278-80-0	47
2			2-Butyne-1,4-diol, bis(.beta.-hy...	174	C8H14O4	001606-85-5	28
3			Oxirane, ethyl-	72	C4H8O	000106-88-7	25
4			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	25
5			2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	25



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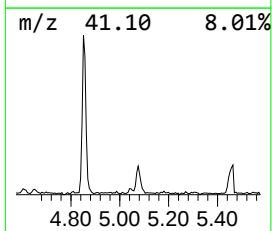
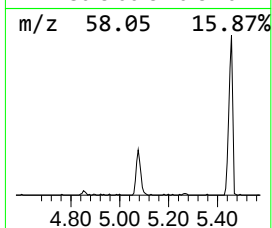
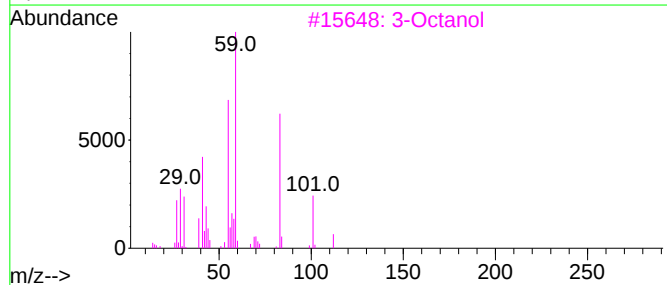
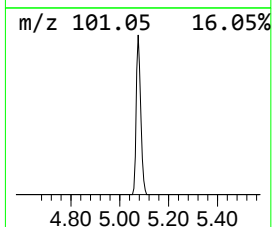
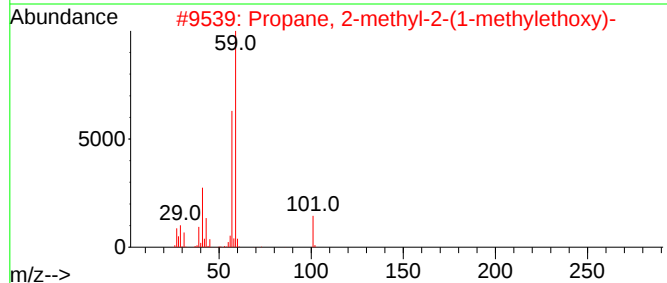
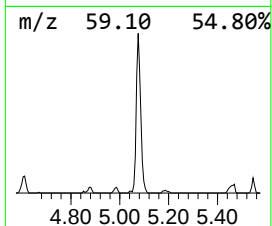
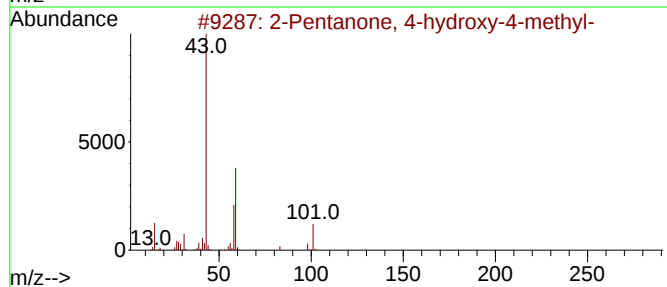
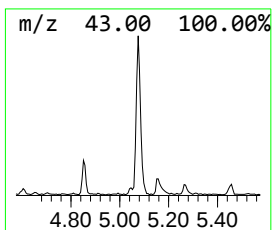
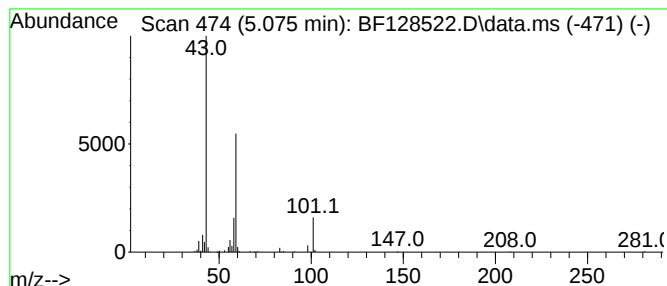
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	2.67 ng	176148	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	50
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Octanol	130	C8H18O	000589-98-0	36
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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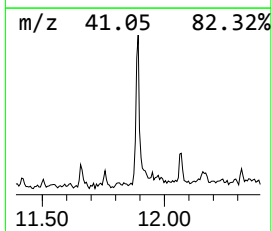
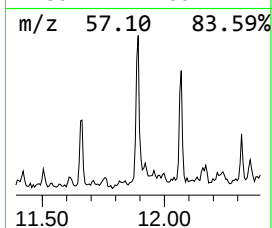
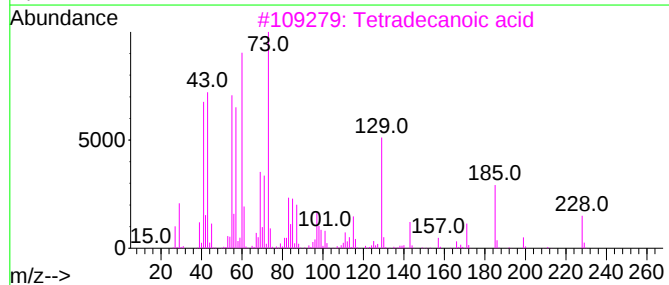
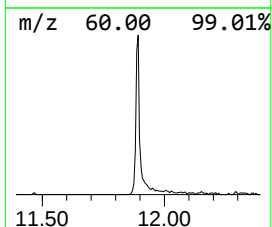
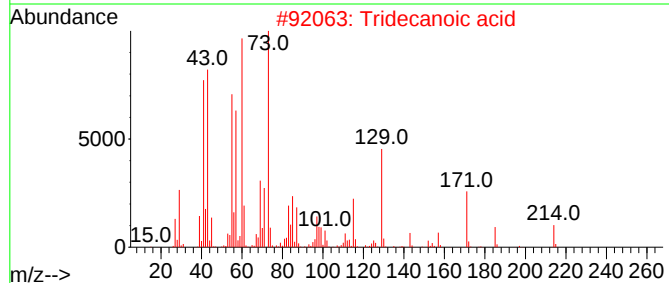
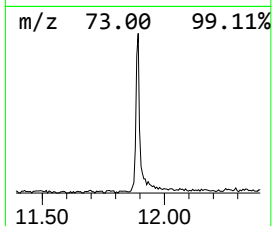
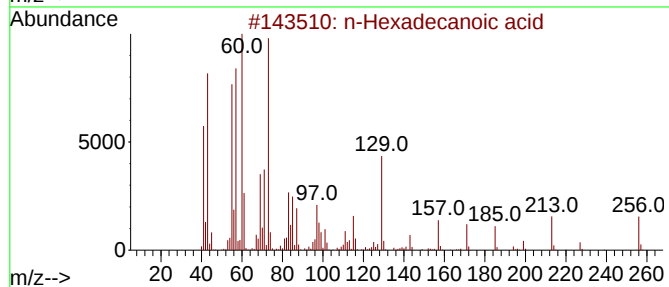
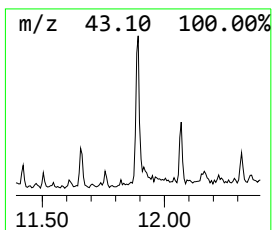
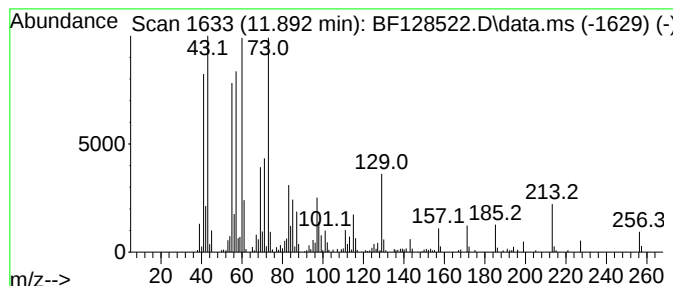
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.892	2.76 ng	248500	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	80
5	Undecanoic acid		186	C11H22O2	000112-37-8	68



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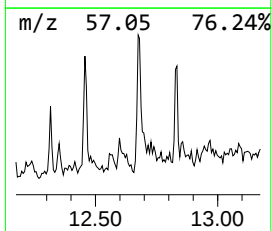
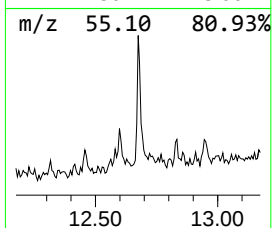
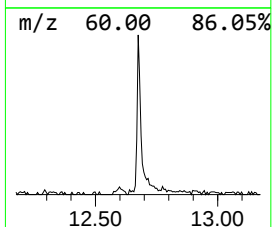
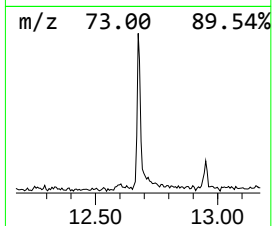
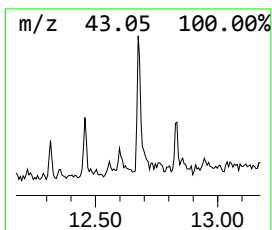
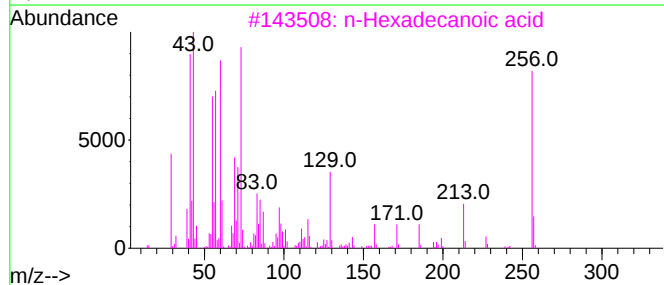
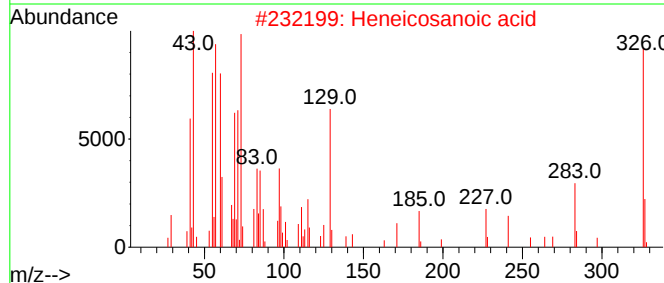
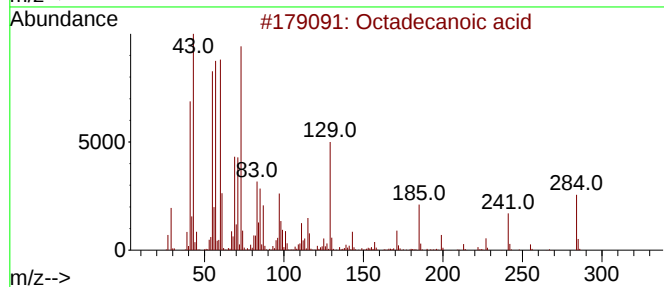
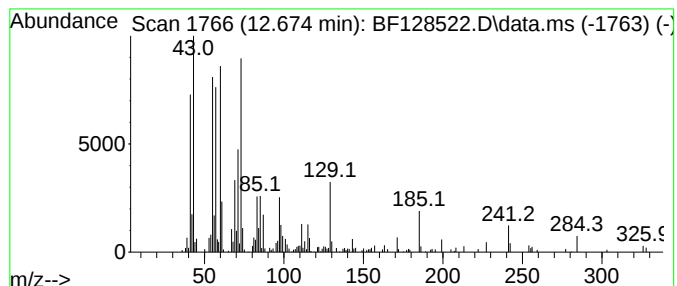
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.675	2.09 ng	188878	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Heneicosanoic acid	326	C21H42O2	002363-71-5	93
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	76



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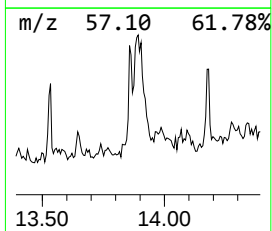
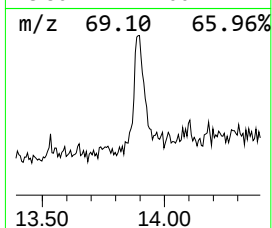
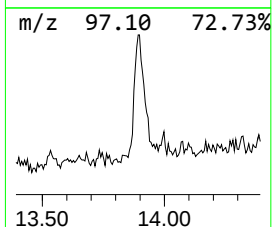
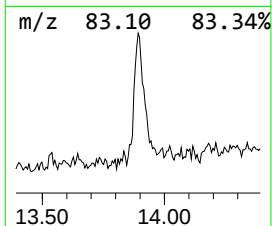
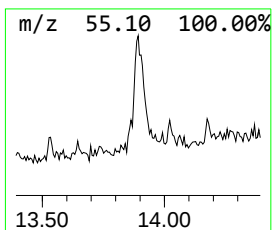
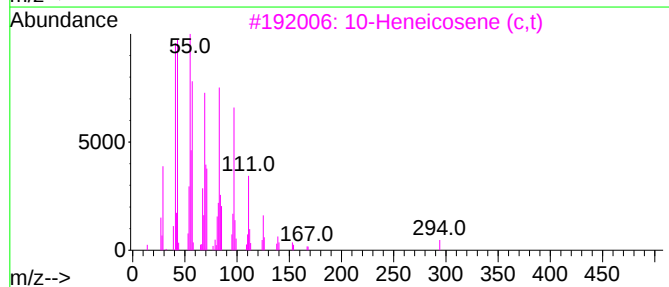
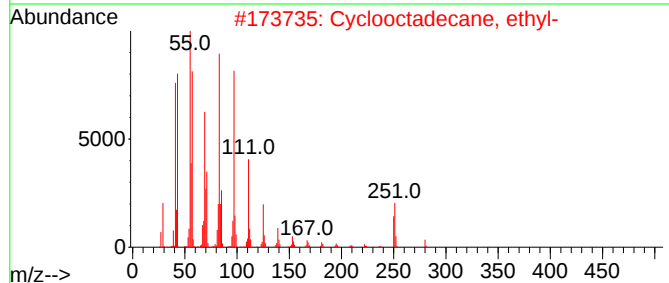
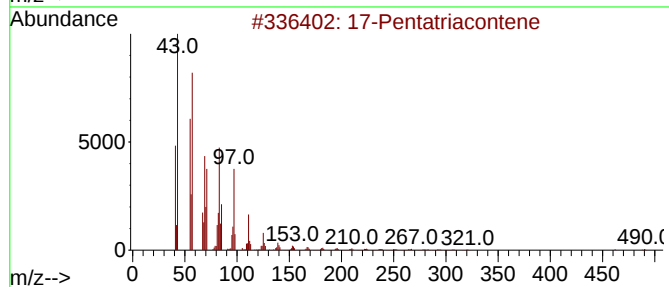
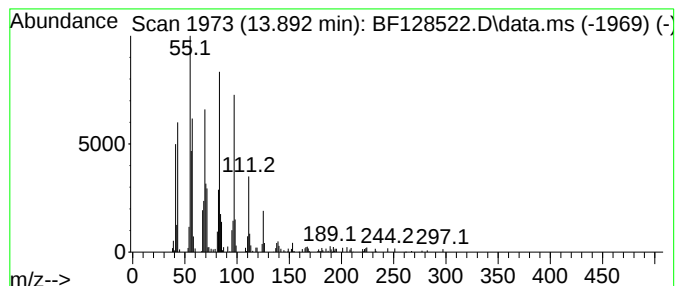
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	5.25 ng	317560	Chrysene-d12	13.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		17-Pentatriacontene	491	C35H70	006971-40-0	87
2		Cyclooctadecane, ethyl-	280	C20H40	1000151-22-5	87
3		10-Heneicosene (c,t)	294	C21H42	095008-11-0	68
4		1-Hexacosanol	382	C26H54O	000506-52-5	64
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128522.D
Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P013-SS002-0006-01

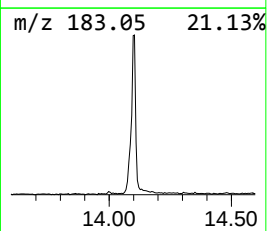
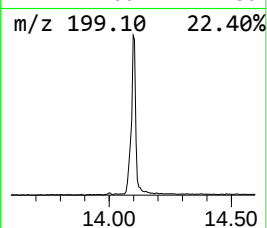
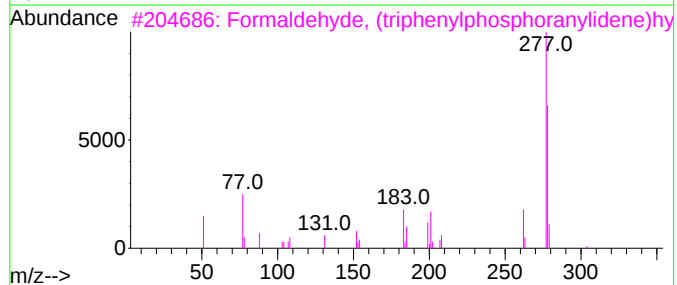
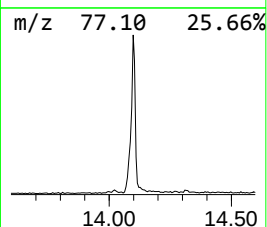
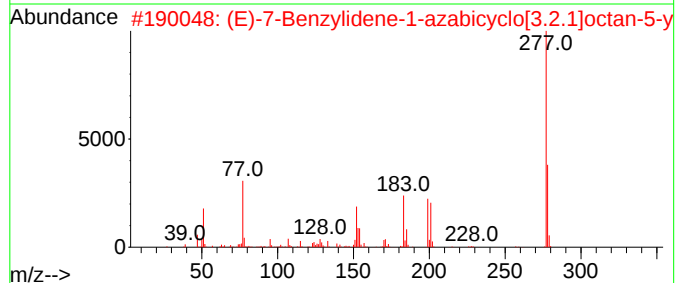
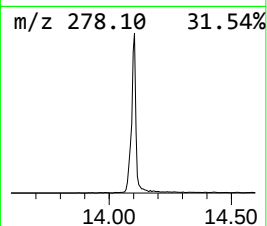
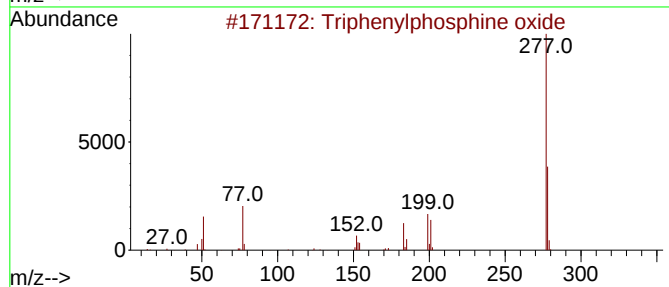
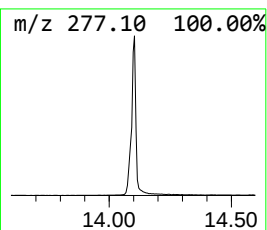
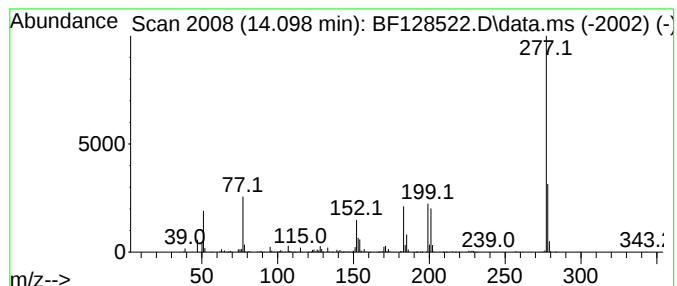
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	20.53 ng	1242250	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	90
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	25
5			Cobalt, (.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
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Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

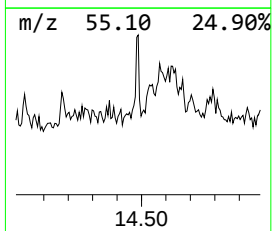
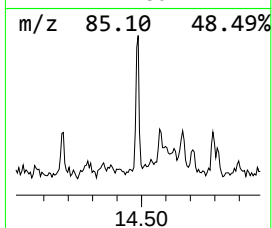
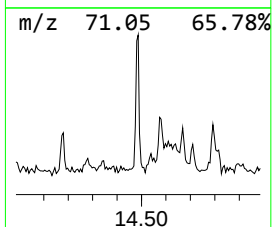
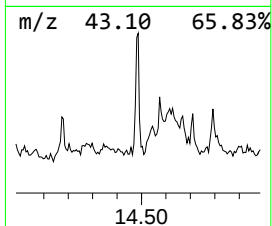
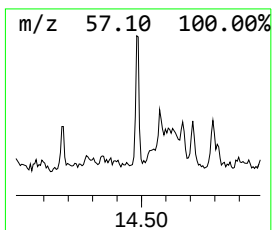
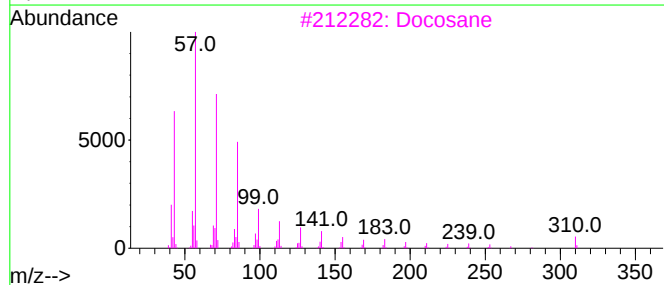
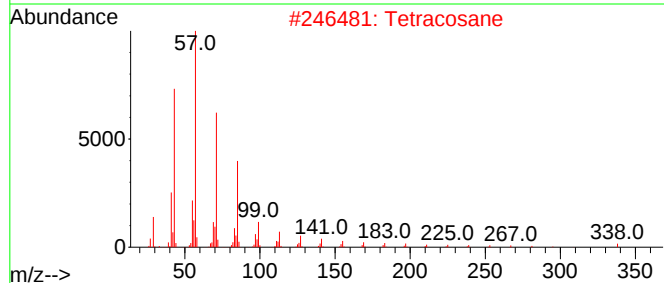
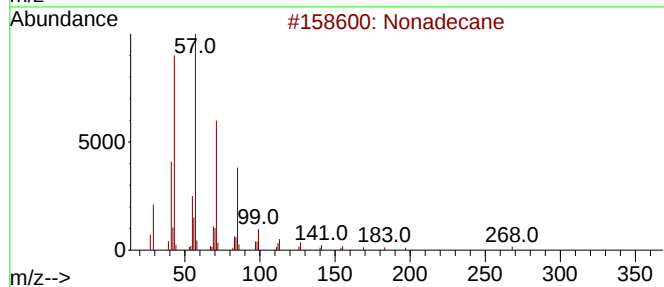
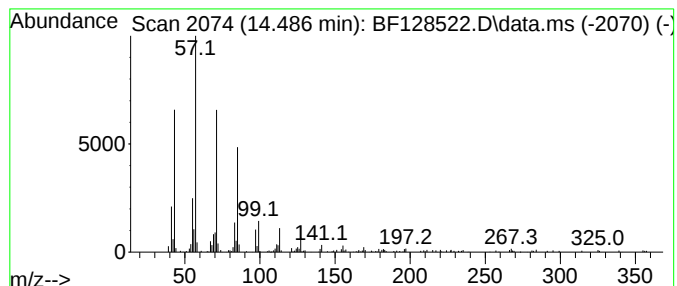
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.486	2.15 ng	129974	Chrysene-d12	13.998	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Docosane	310	C22H46	000629-97-0	86
4	Heptadecane	240	C17H36	000629-78-7	86
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128522.D
Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P013-SS002-0006-01

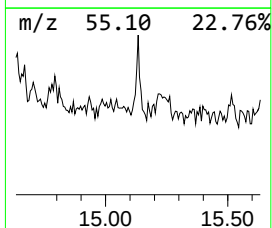
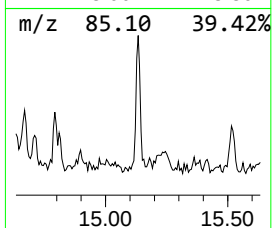
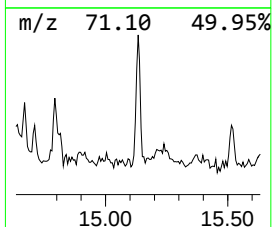
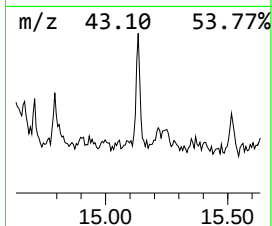
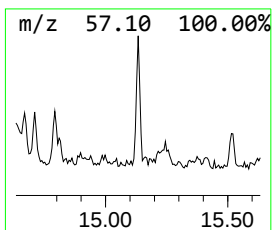
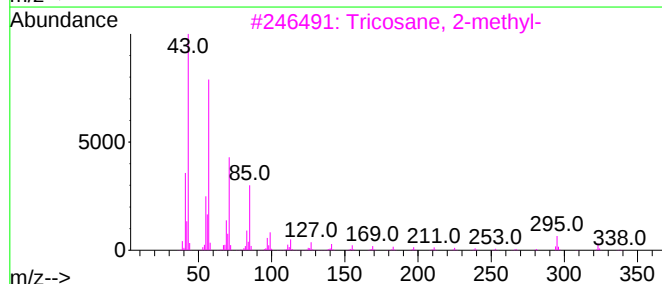
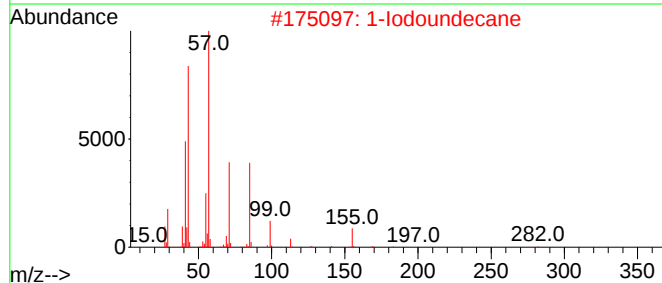
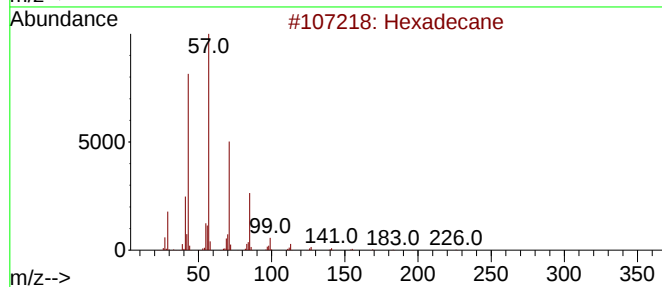
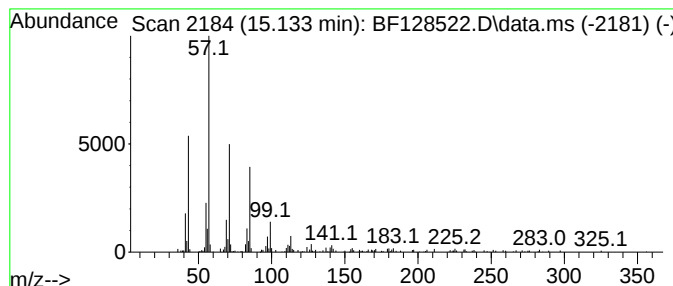
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	2.56 ng	132311	Perylene-d12	15.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	90
2			1-Iodoundecane	282	C11H23I	004282-44-4	87
3			Tricosane, 2-methyl-	338	C24H50	001928-30-9	86
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
5			Undecane, 3-methyl-	170	C12H26	001002-43-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128522.D
Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

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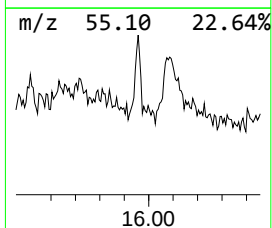
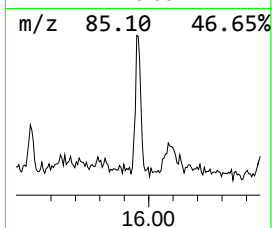
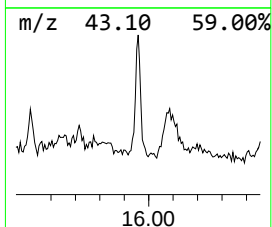
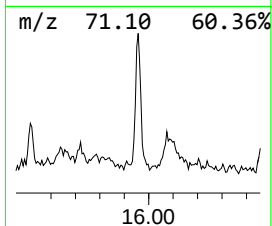
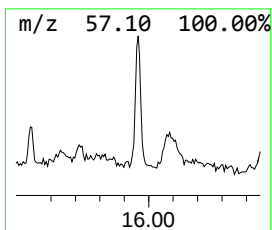
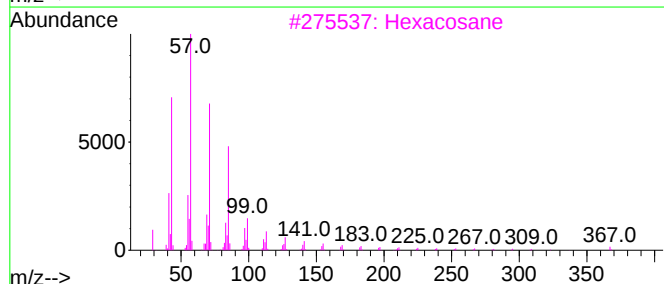
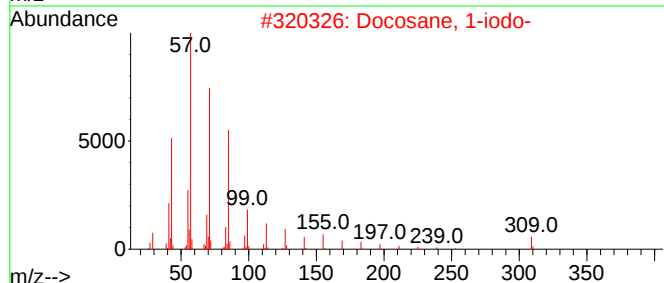
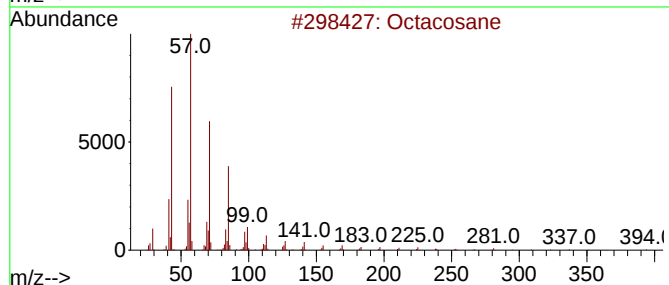
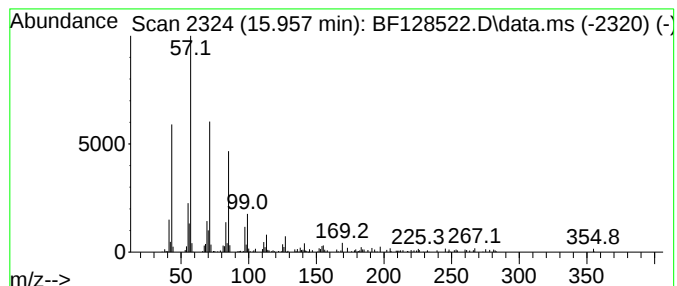
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.957	2.91 ng	150622	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
3		Hexacosane	366	C26H54	000630-01-3	86
4		Tetracosane	338	C24H50	000646-31-1	86
5		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
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Misc :
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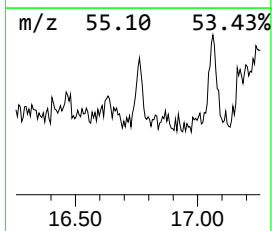
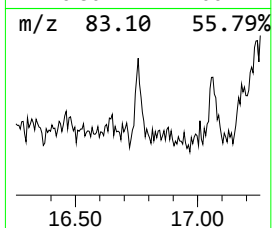
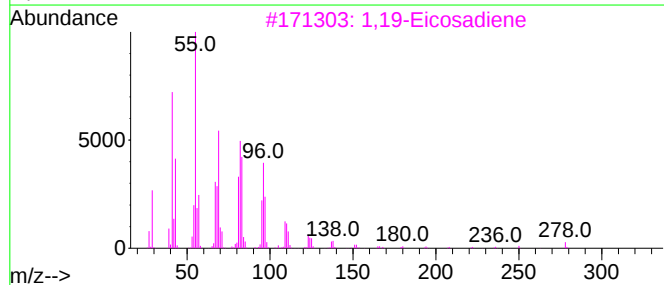
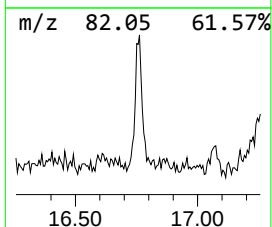
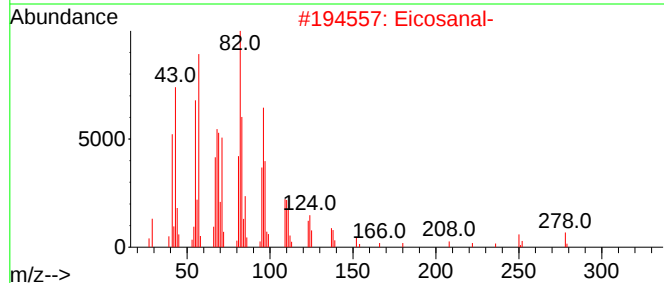
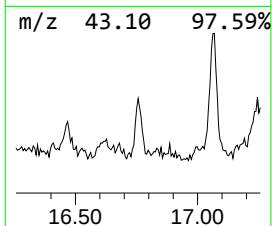
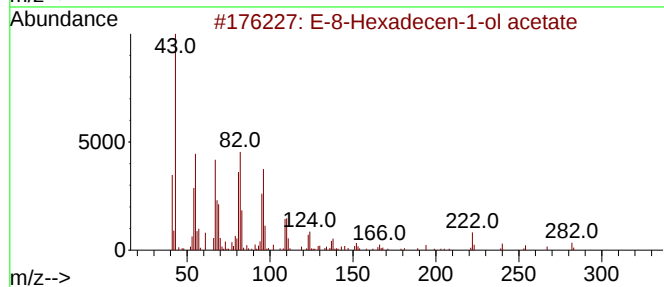
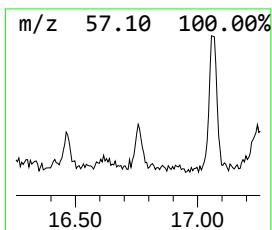
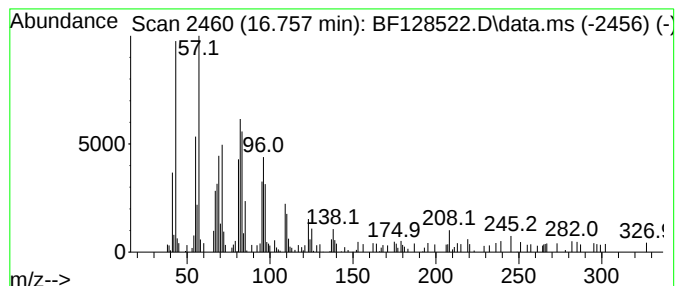
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 E-8-Hexadecen-1-ol acetate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.757	2.05 ng	106318	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-8-Hexadecen-1-ol acetate	282	C18H34O2	1000131-01-1	64
2	Eicosanal-	296	C20H40O	002400-66-0	58
3	1,19-Eicosadiene	278	C20H38	014811-95-1	52
4	1-Eicosyne	278	C20H38	000765-27-5	50
5	1-Cyclohexylnonene	208	C15H28	114614-84-5	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
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ALS Vial : 10 Sample Multiplier: 1

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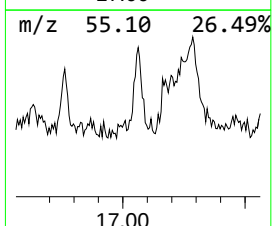
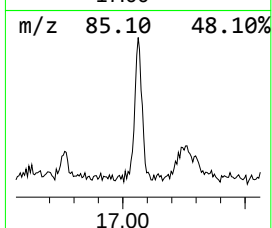
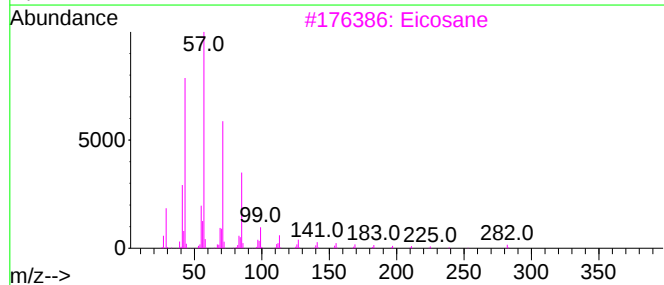
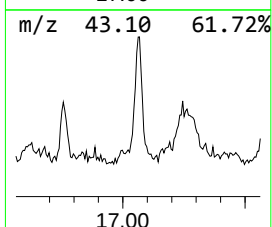
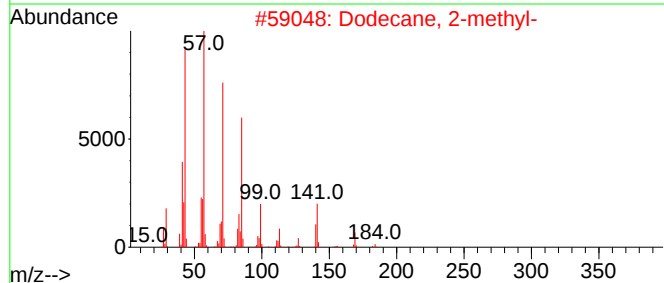
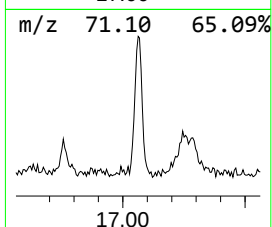
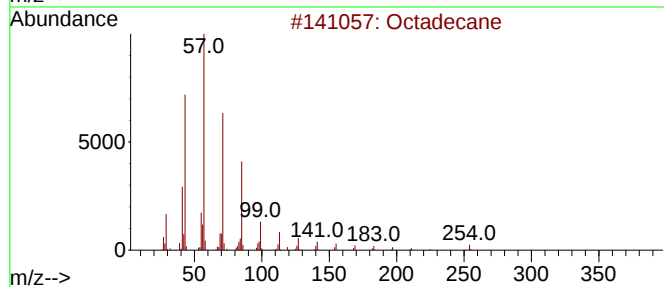
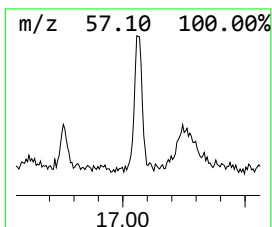
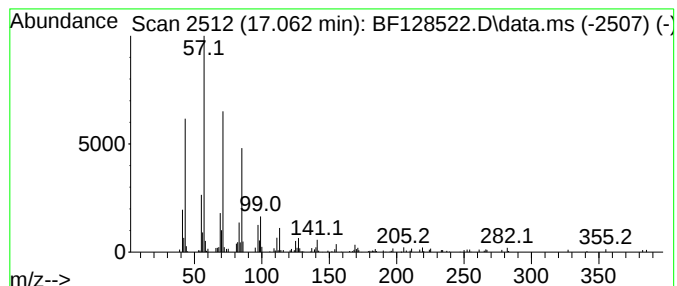
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.062	4.00 ng	206978	Perylene-d12	15.463

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecane	254	C18H38	000593-45-3	95
2		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
3		Eicosane	282	C20H42	000112-95-8	89
4		Docosane, 11-decyl-	451	C32H66	055401-55-3	87
5		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128522.D
Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

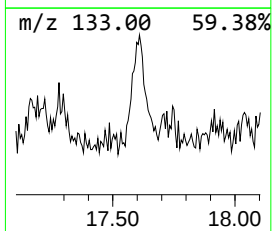
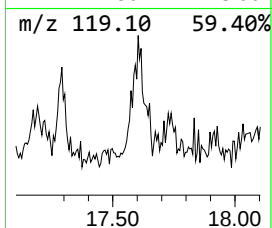
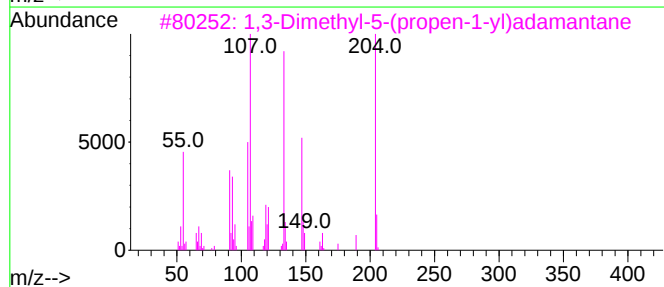
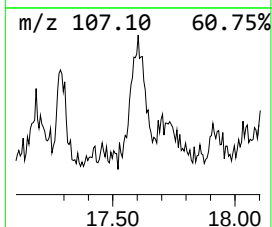
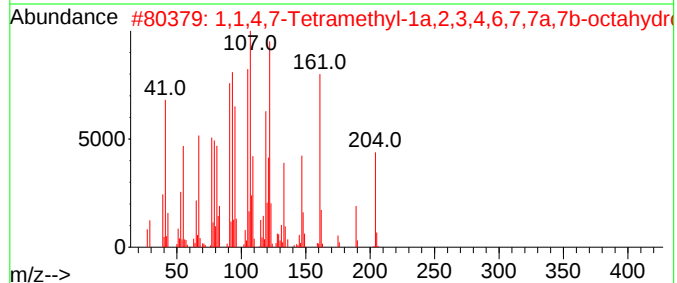
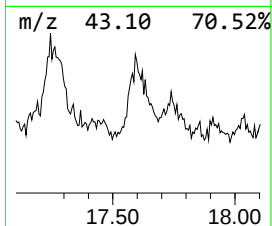
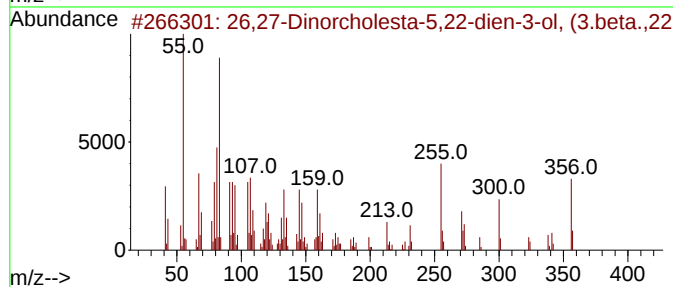
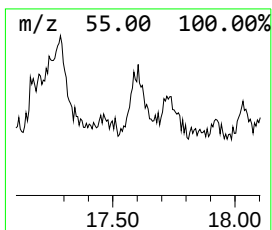
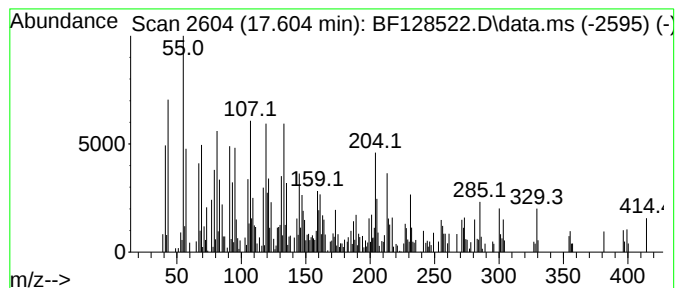
Instrument :
BNA_F
ClientSampleId :
P013-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown17.604 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.604	7.32 ng	378979	Perylene-d12	15.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	49
2	1,1,4,7-Tetramethyl-1a,2,3,4,6,7...	204	C15H24	405112-35-8	47
3	1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	45
4	(1S,2E,4E,7E,10R,11E)-10-Acetoxy...	330	C22H34O2	1000433-18-1	38
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052722\
Data File : BF128522.D
Acq On : 27 May 2022 21:29
Operator : CG\JU
Sample : N2921-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P013-SS002-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.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
1-Pentene, 3-et...	4.410	2.2	ng	144646	1	6.840	1319180	20.0
unknown4.851	4.851	2.4	ng	156246	1	6.840	1319180	20.0
2-Pentanone, 4-...	5.075	2.7	ng	176148	1	6.840	1319180	20.0
n-Hexadecanoic ...	11.892	2.8	ng	248500	4	11.363	1803480	20.0
Octadecanoic acid	12.675	2.1	ng	188878	4	11.363	1803480	20.0
17-Pentatriacon...	13.892	5.3	ng	317560	5	13.998	1210340	20.0
Triphenylphosph...	14.098	20.5	ng	1242250	5	13.998	1210340	20.0
Nonadecane	14.486	2.1	ng	129974	5	13.998	1210340	20.0
Hexadecane	15.133	2.6	ng	132311	6	15.463	1034930	20.0
Octacosane	15.957	2.9	ng	150622	6	15.463	1034930	20.0
E-8-Hexadecen-1...	16.757	2.0	ng	106318	6	15.463	1034930	20.0
Octadecane	17.062	4.0	ng	206978	6	15.463	1034930	20.0
unknown17.604	17.604	7.3	ng	378979	6	15.463	1034930	20.0