

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
 Data File : BF128758.D
 Acq On : 10 Jun 2022 14:50
 Operator : CG\JU
 Sample : N3287-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128758.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.004	459	462	467	rVB	42889	46124	1.67%	0.298%
2	5.445	534	537	544	rBV	910769	833966	30.27%	5.382%
3	6.463	706	710	719	rBV	528436	503911	18.29%	3.252%
4	6.798	763	767	771	rVB	539832	441792	16.03%	2.851%
5	7.369	858	864	867	rBV	1448102	1453600	52.75%	9.381%
6	8.086	981	986	989	rVB	651397	577855	20.97%	3.729%
7	9.163	1163	1169	1172	rBV	2832484	2755503	100.00%	17.782%
8	9.839	1279	1284	1288	rBV	752658	668094	24.25%	4.311%
9	10.480	1385	1393	1399	rVB	19965	51237	1.86%	0.331%
10	10.633	1415	1419	1428	rBV	1432363	1326324	48.13%	8.559%
11	11.327	1533	1537	1541	rBV	739753	685175	24.87%	4.422%
12	11.851	1622	1626	1637	rBV2	134283	234003	8.49%	1.510%
13	12.004	1649	1652	1657	rVB2	56049	74118	2.69%	0.478%
14	12.069	1660	1663	1672	rVB8	27436	52306	1.90%	0.338%
15	12.504	1734	1737	1741	rBV	36858	43301	1.57%	0.279%
16	12.645	1741	1761	1774	rVV	733583	1331543	48.32%	8.593%
17	12.921	1803	1808	1811	rBV	2708006	2314956	84.01%	14.939%
18	13.321	1871	1876	1883	rVB3	36384	75084	2.72%	0.485%
19	13.974	1983	1987	1990	rBV	461878	409887	14.88%	2.645%
20	14.004	1990	1992	1997	rVB	80702	104064	3.78%	0.672%
21	14.068	1998	2003	2009	rBV	296784	302145	10.97%	1.950%
22	14.557	2082	2086	2092	rVV	110198	150998	5.48%	0.974%
23	14.933	2145	2150	2160	rVB7	54521	118680	4.31%	0.766%
24	15.104	2175	2179	2187	rVB	80586	153837	5.58%	0.993%
25	15.433	2230	2235	2243	rVB	329102	436192	15.83%	2.815%
26	15.733	2281	2286	2294	rBV2	49002	96613	3.51%	0.623%
27	16.209	2361	2367	2381	rVB6	64889	184963	6.71%	1.194%
28	16.462	2406	2410	2416	rVB4	31925	69451	2.52%	0.448%

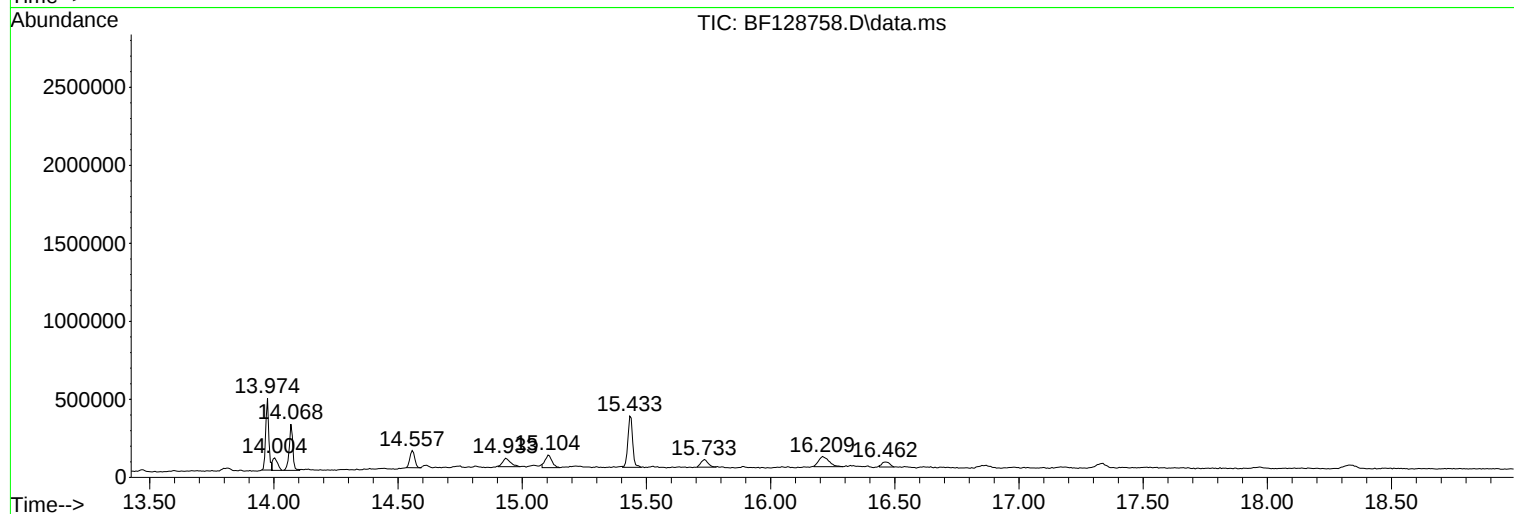
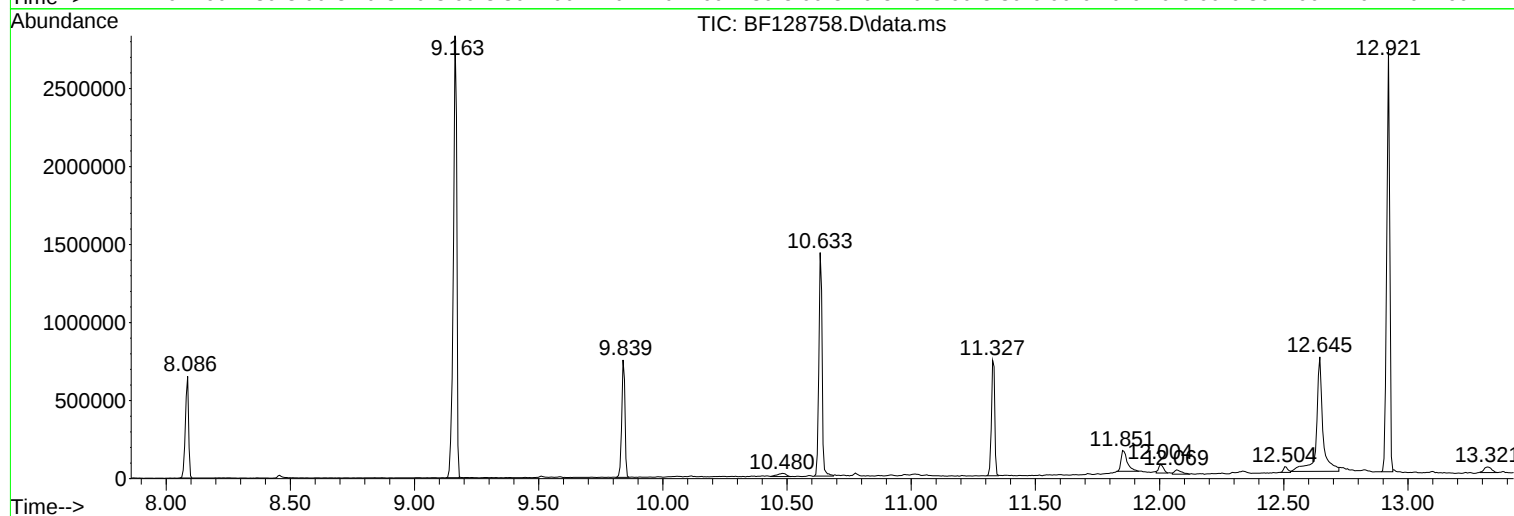
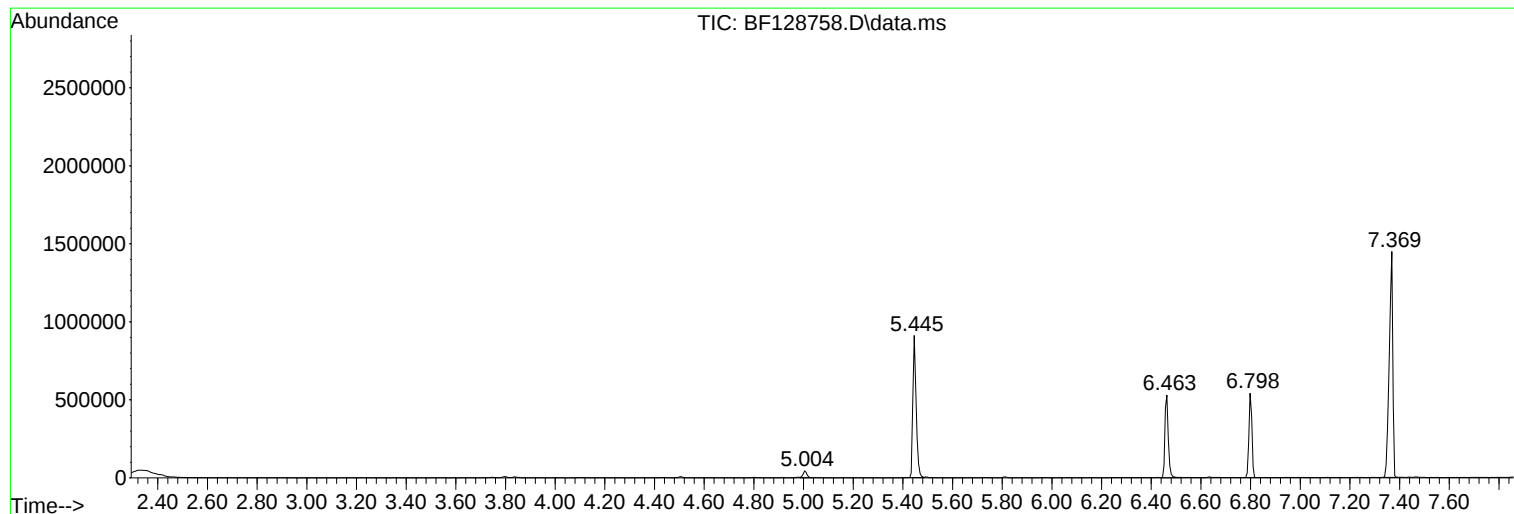
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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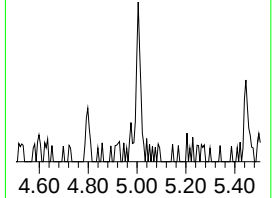
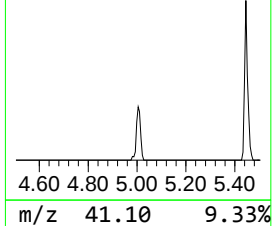
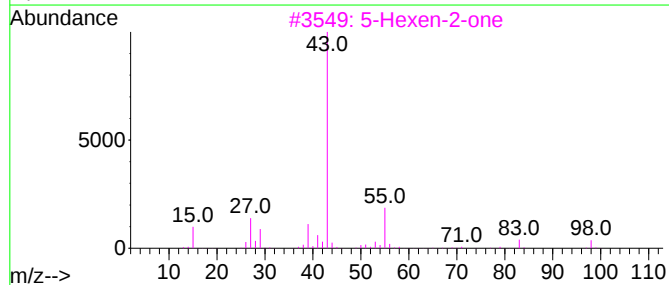
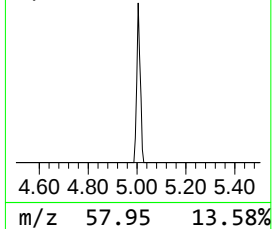
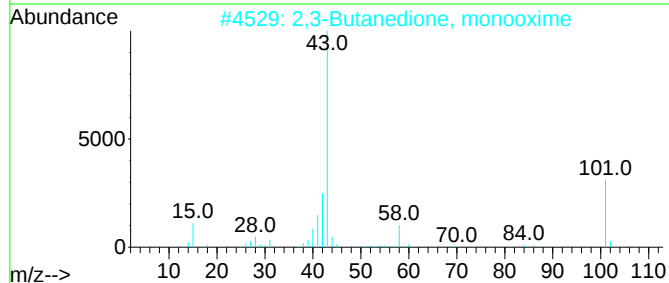
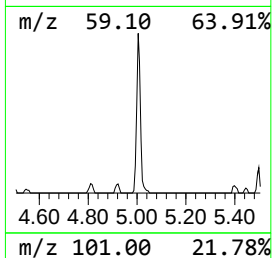
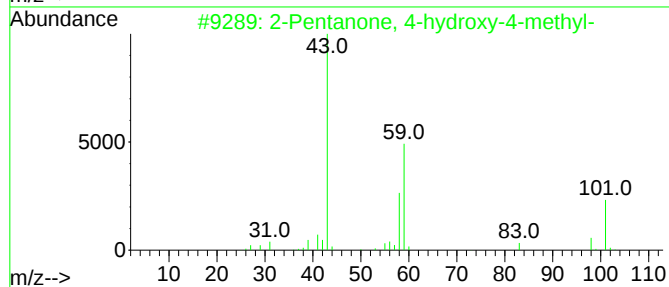
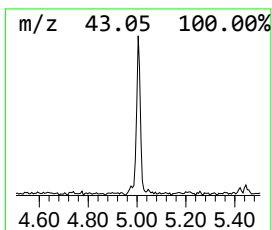
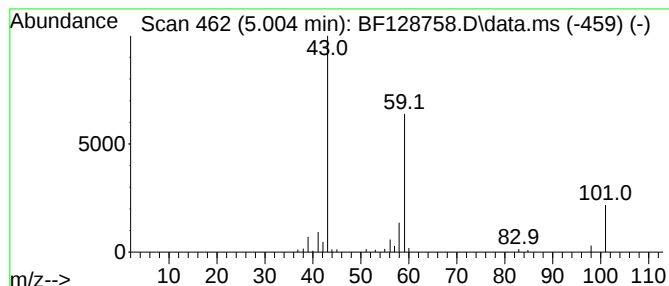
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.004	2.09 ng	46124	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3			5-Hexen-2-one	98	C6H10O	000109-49-9	9
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5			Pentanal, oxime	101	C5H11NO	000628-79-5	9



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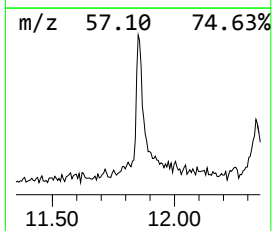
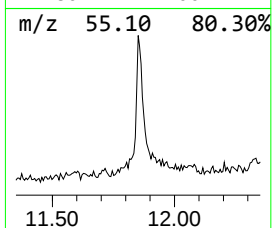
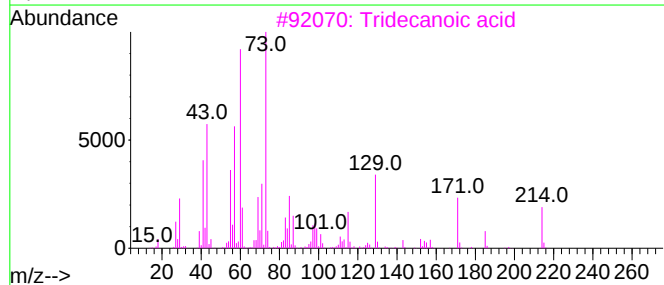
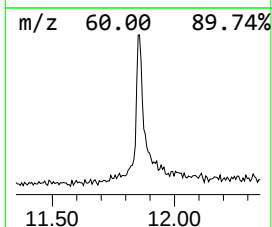
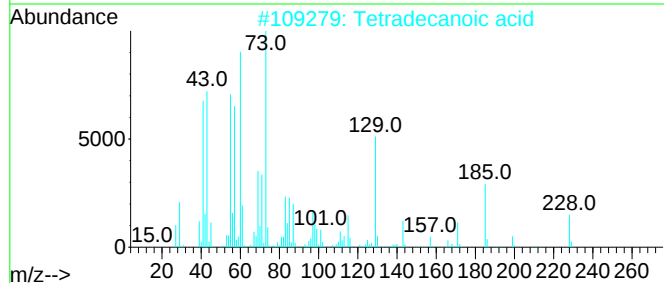
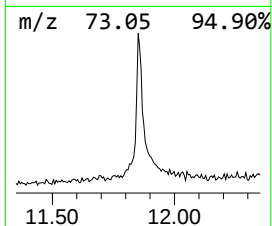
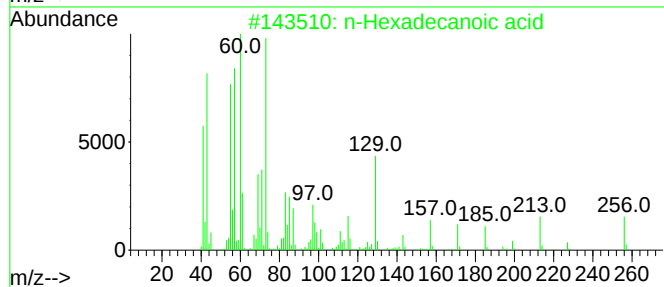
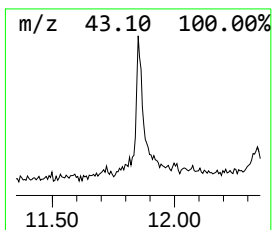
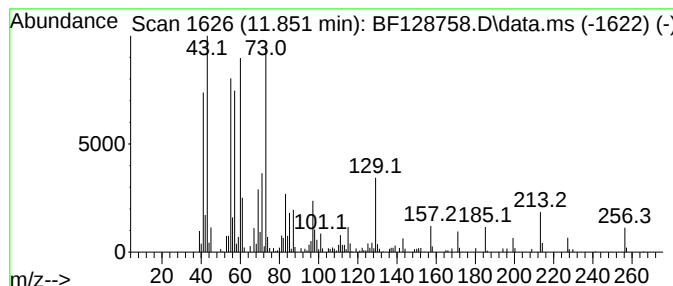
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	6.83 ng	234003	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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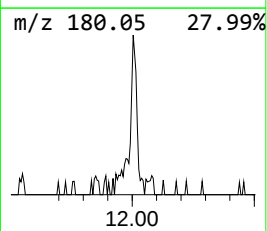
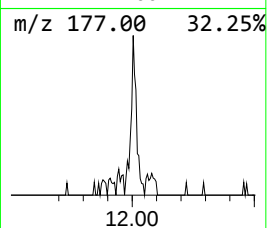
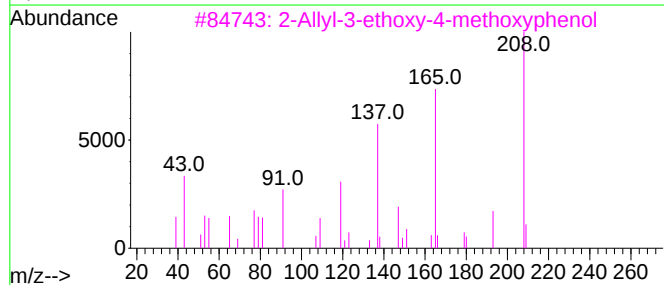
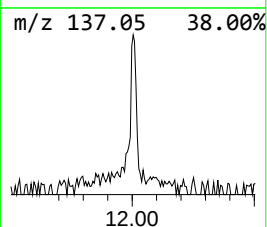
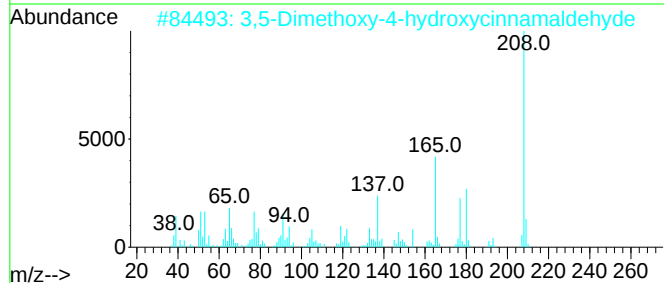
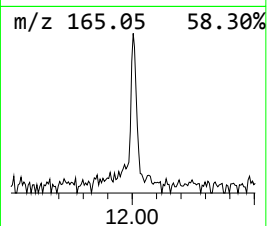
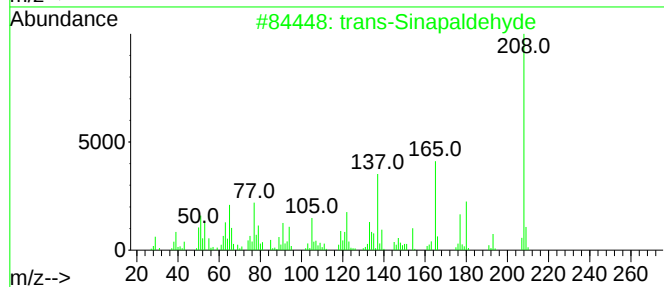
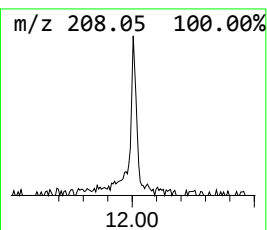
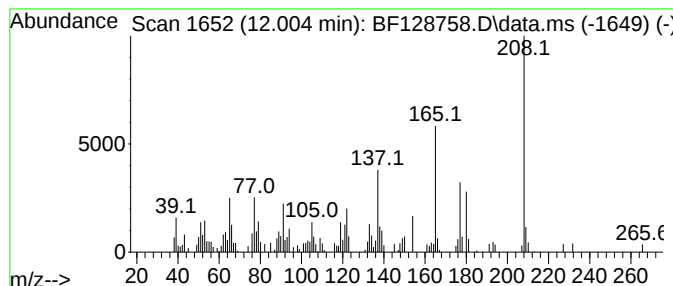
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 trans-Sinapaldehyde Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	2.16 ng	74118	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Sinapaldehyde	208	C11H12O4	004206-58-0	93
2			3,5-Dimethoxy-4-hydroxycinnamaldehyde	208	C11H12O4	087345-53-7	91
3			2-Allyl-3-ethoxy-4-methoxyphenol	208	C12H16O3	1000122-70-6	64
4			Coumarin, 7,8-dihydro-7-hydroxy-	208	C10H8O5	1000263-13-6	58
5			2-Propenoic acid, 3-(2,3-dimethoxy-5-hydroxyphenyl)-	208	C11H12O4	007345-82-6	50



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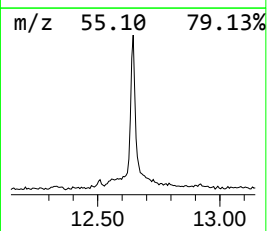
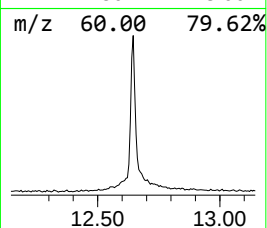
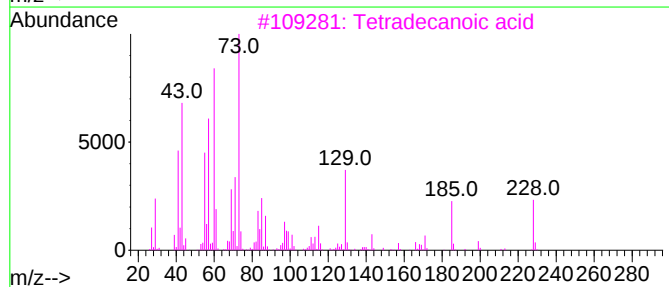
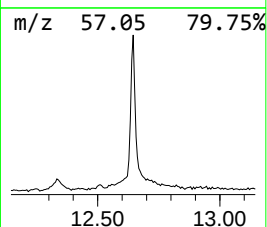
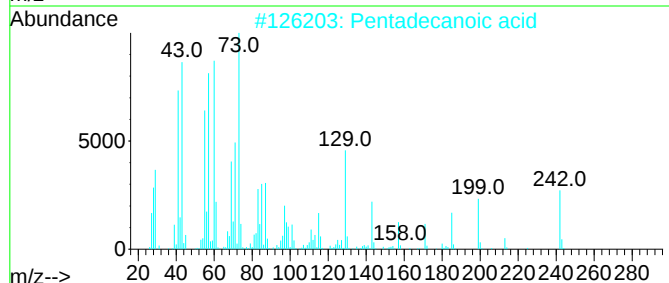
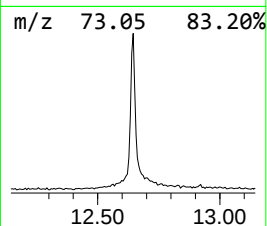
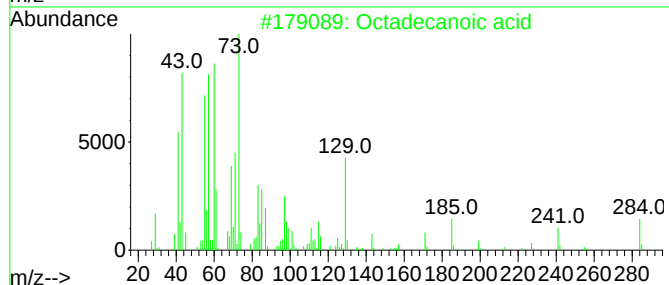
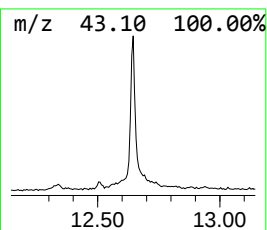
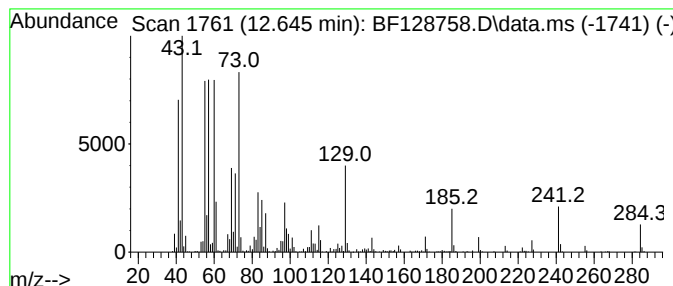
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.645	38.87 ng	1331540	Phenanthrene-d10	11.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64



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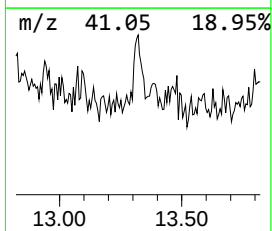
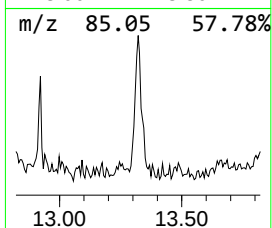
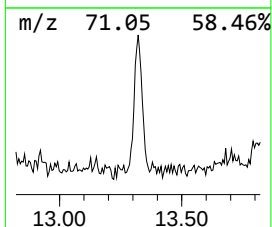
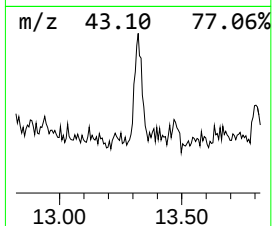
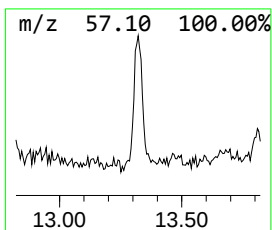
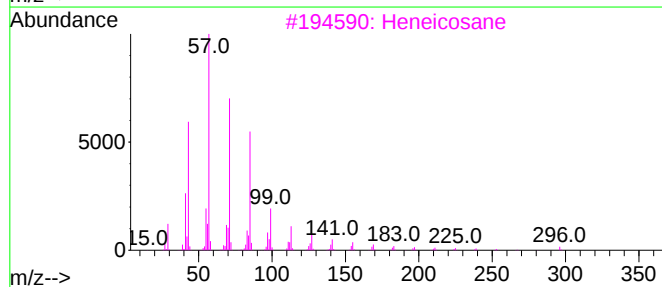
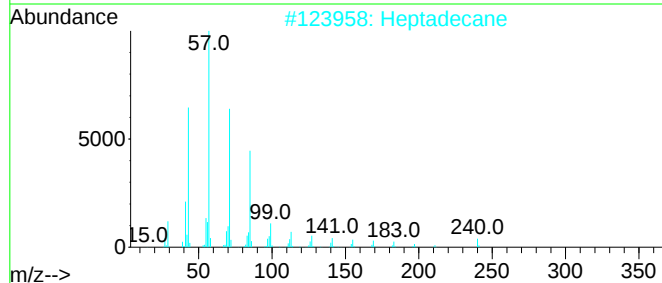
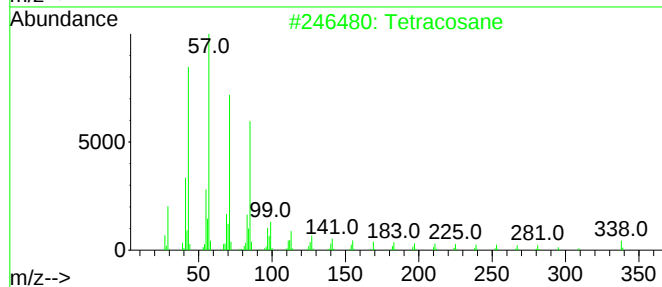
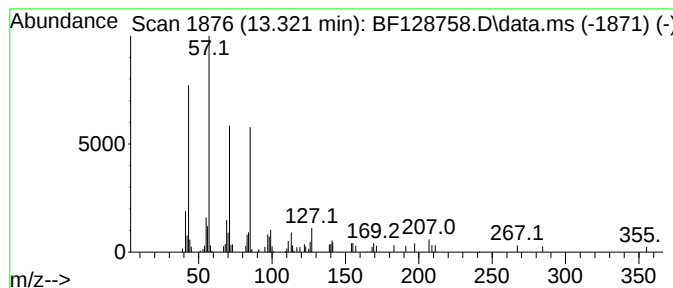
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Tetracosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.321	3.66 ng	75084	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	86
2			Heptadecane	240	C17H36	000629-78-7	86
3			Heneicosane	296	C21H44	000629-94-7	83
4			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	80
5			Nonadecane	268	C19H40	000629-92-5	80



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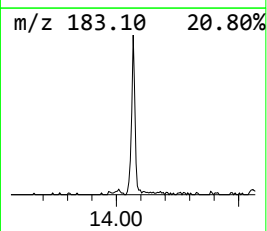
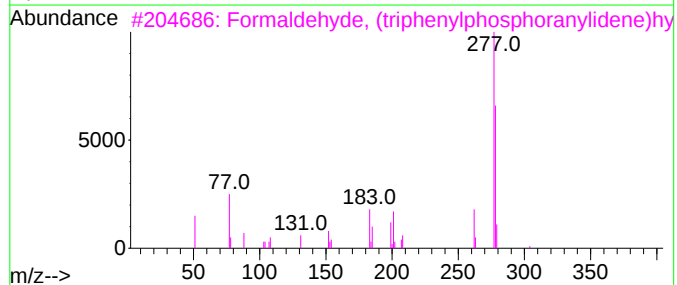
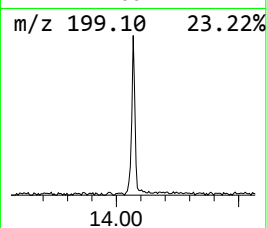
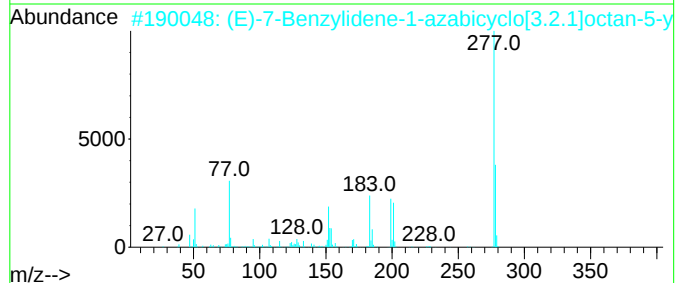
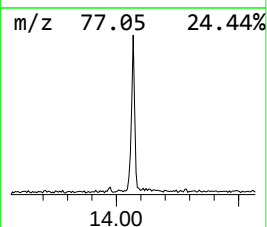
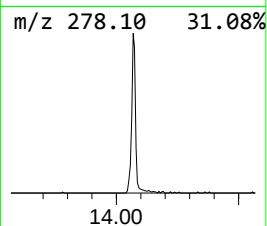
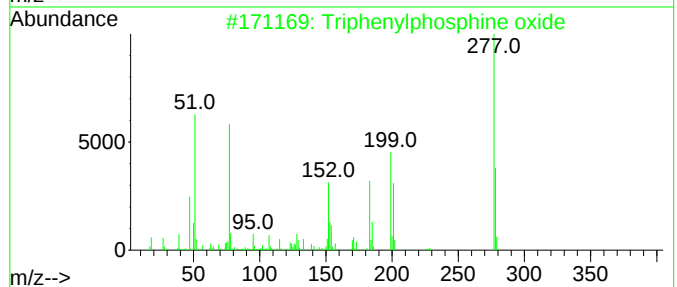
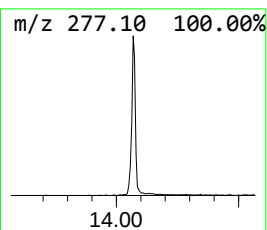
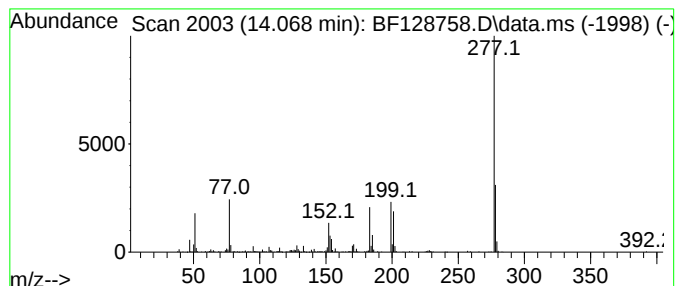
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Triphenylphosphine oxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.068	14.74 ng	302145	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	70
3			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	40
5			3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
Operator : CG\JU
Sample : N3287-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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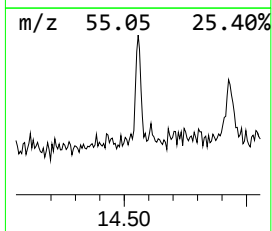
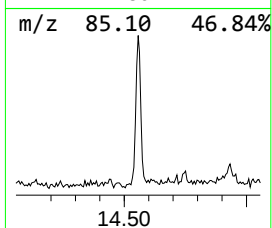
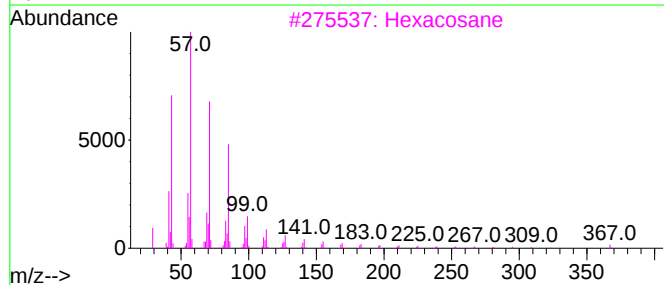
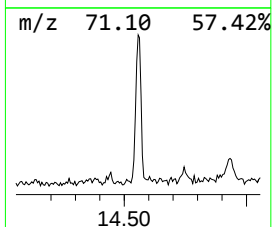
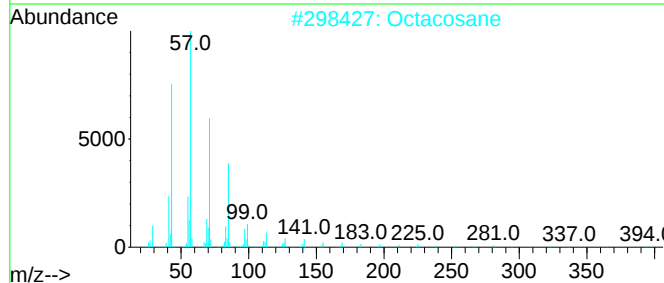
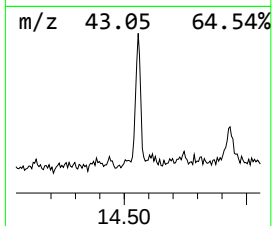
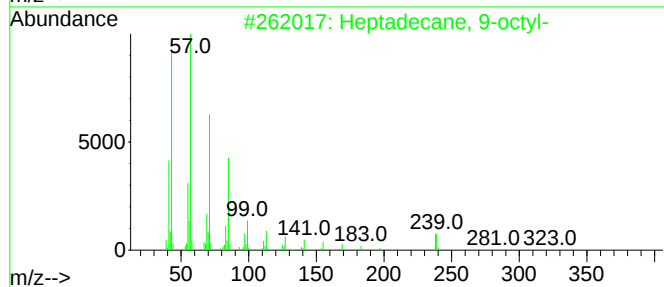
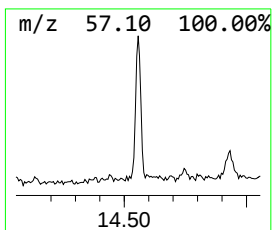
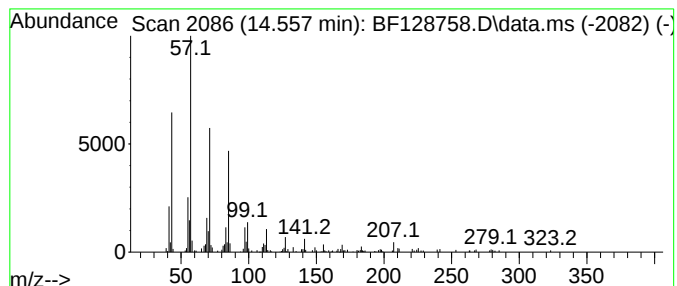
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	7.37 ng	150998	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
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Misc :
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Instrument :
BNA_F
ClientSampleId :
MW-1

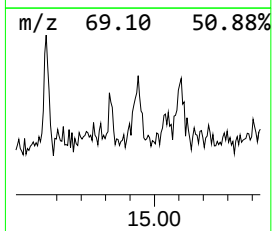
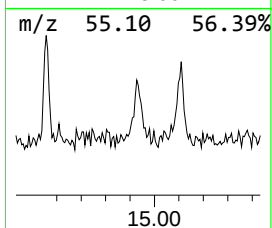
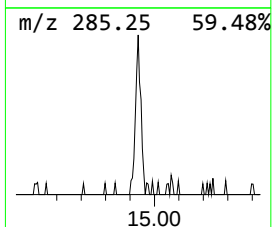
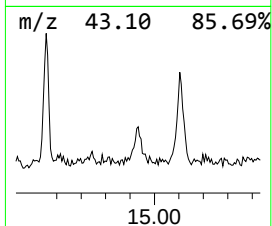
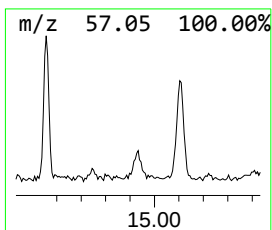
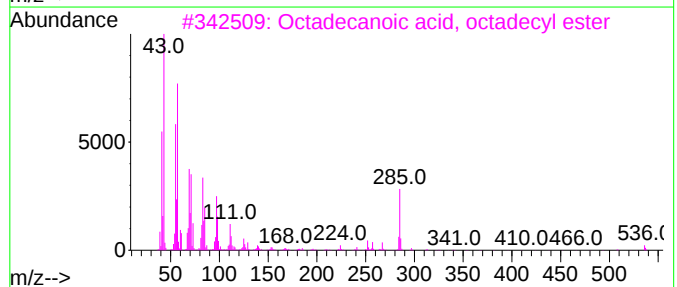
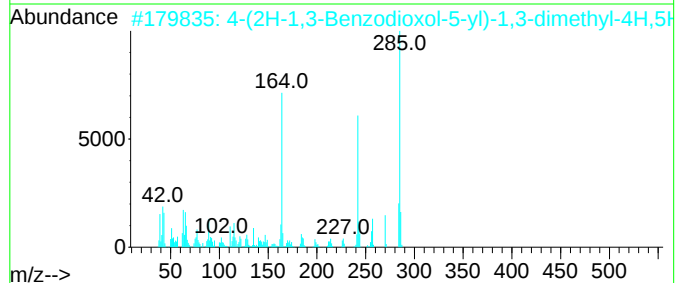
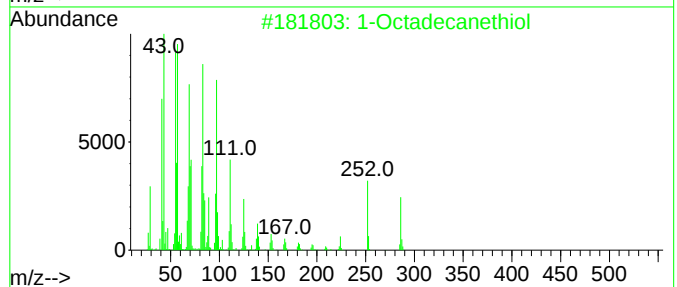
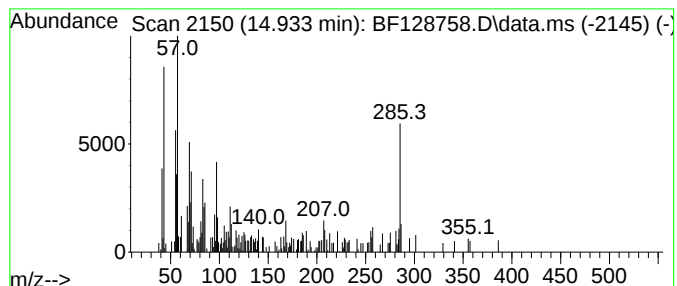
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.933 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.933	5.44 ng	118680	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanethiol	286	C18H38S	002885-00-9	38
2			4-(2H-1,3-Benzodioxol-5-yl)-1,3-...	285	C15H15N3O3	1000388-03-4	25
3			Octadecanoic acid, octadecyl ester	537	C36H72O2	002778-96-3	22
4			Methyl 4-(1-methyl-6-oxo-4H,5H,7...	285	C15H15N3O3	1000388-59-4	18
5			dibenz[c,e][1,2]azaborine, 5,6-d...	285	C19H16BNO	1000397-24-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
Operator : CG\JU
Sample : N3287-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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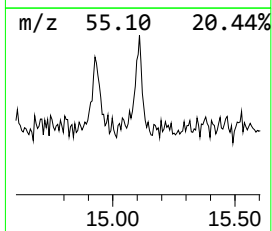
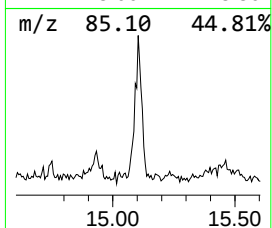
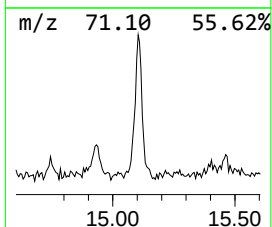
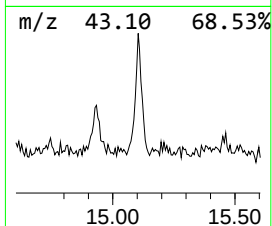
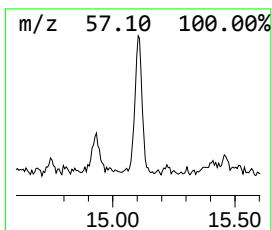
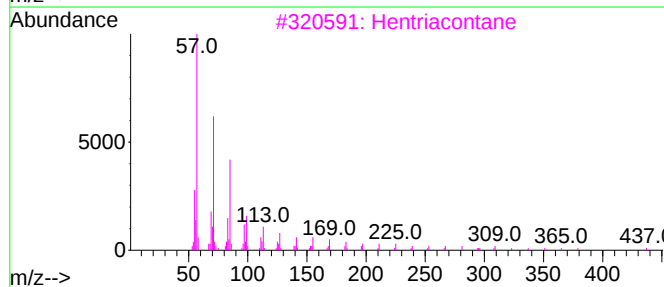
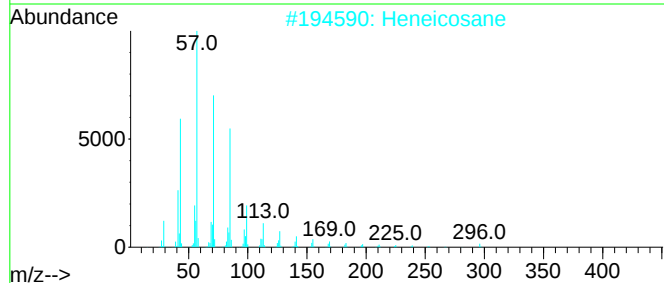
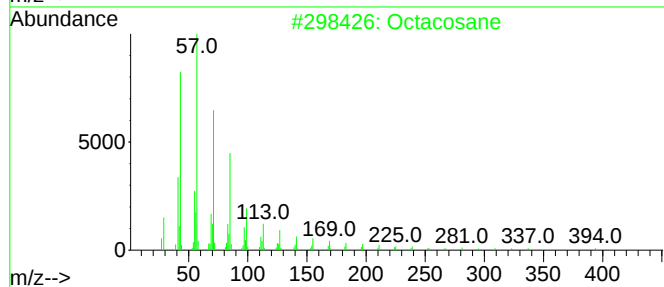
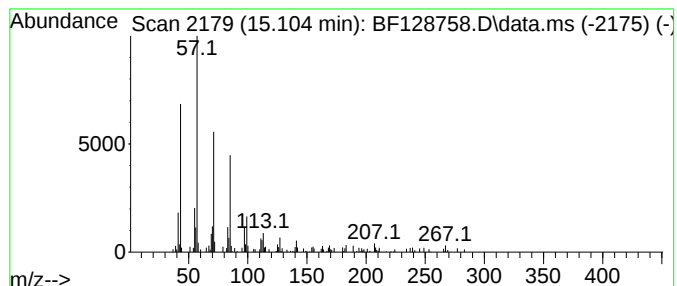
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	7.05 ng	153837	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Hexatriacontane	507	C36H74	000630-06-8	87
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
Operator : CG\JU
Sample : N3287-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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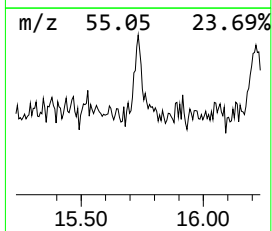
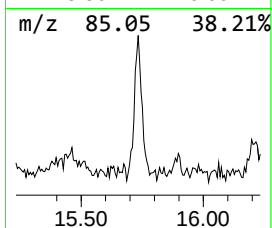
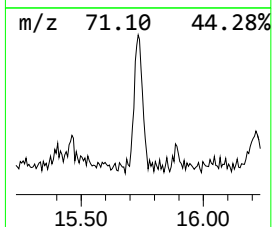
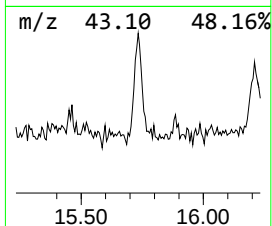
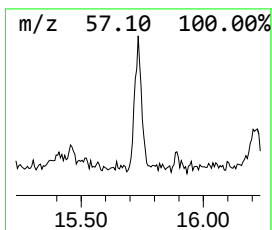
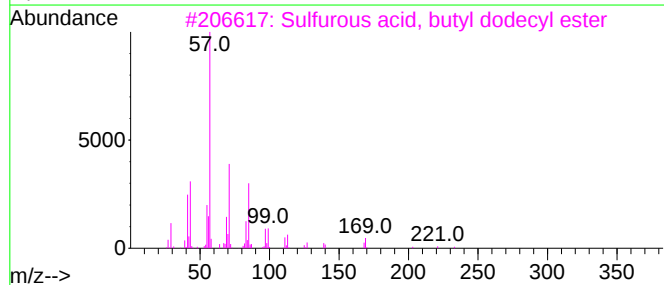
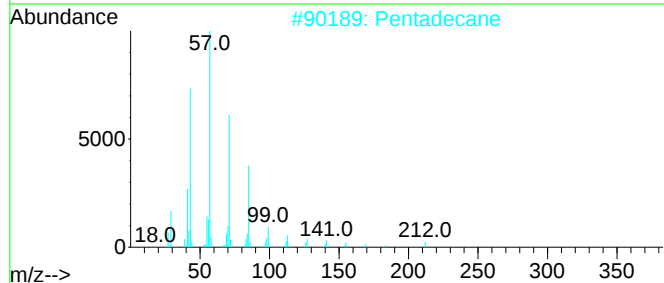
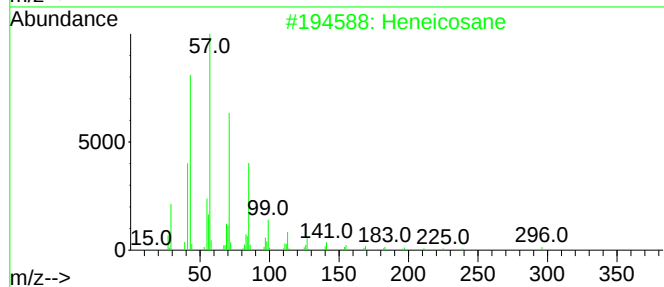
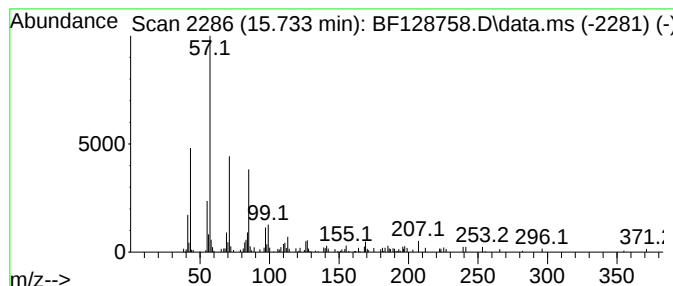
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.733	4.43 ng	96613	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Pentadecane	212	C15H32	000629-62-9	91
3			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
4			1-Iodoundecane	282	C11H23I	004282-44-4	76
5			Eicosane, 2-methyl-	296	C21H44	001560-84-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

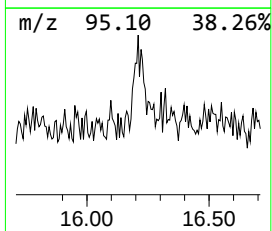
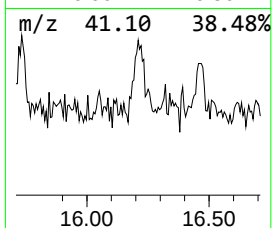
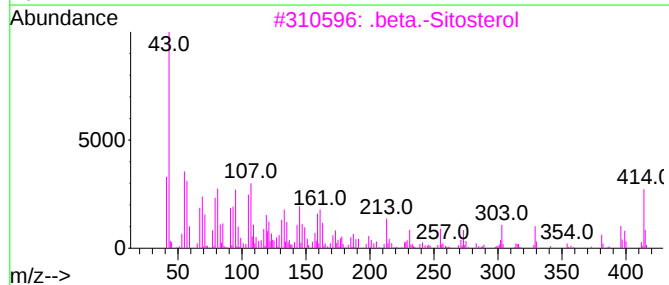
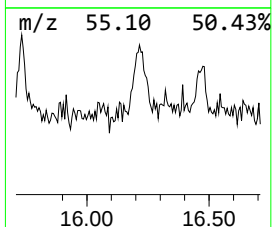
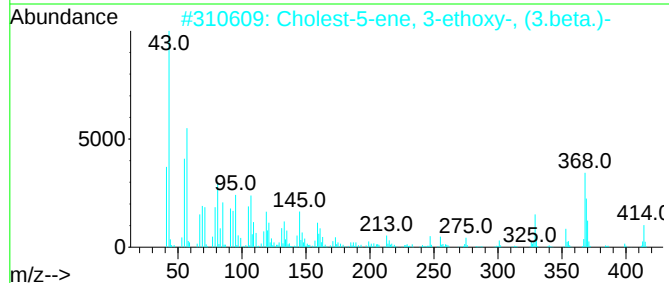
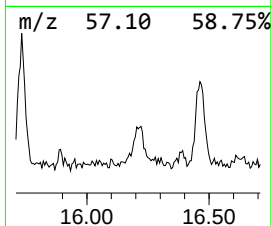
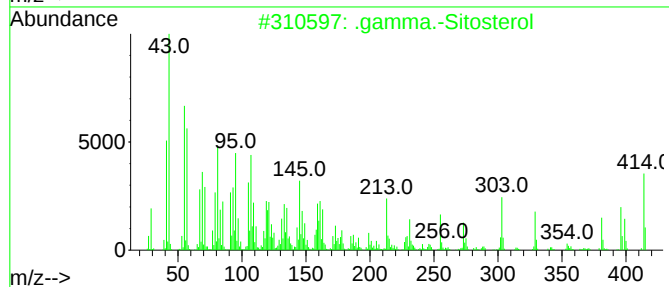
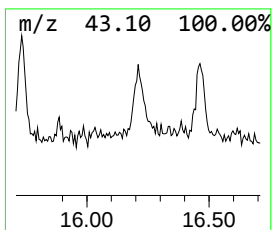
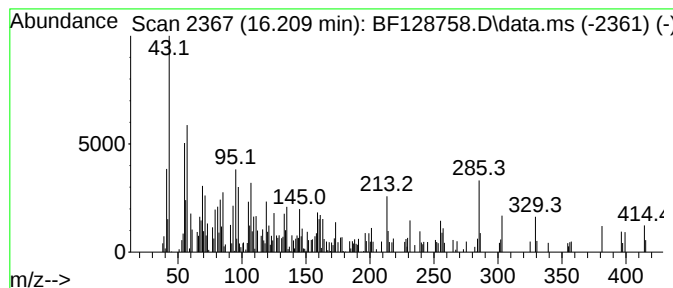
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.209	8.48 ng	184963	Perylene-d12	15.433

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	92
2		Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	91
3		.beta.-Sitosterol	414	C29H50O	000083-46-5	43
4		I-22,23-Dihydrostigmasterol	414	C29H50O	1000214-82-6	35
5		.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
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Sample : N3287-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

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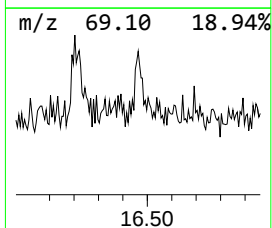
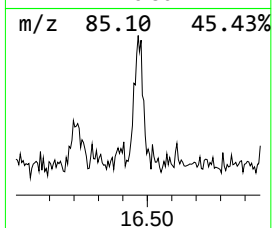
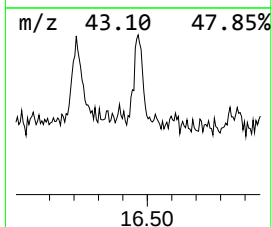
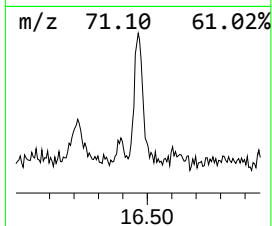
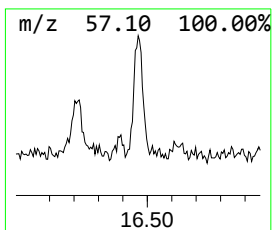
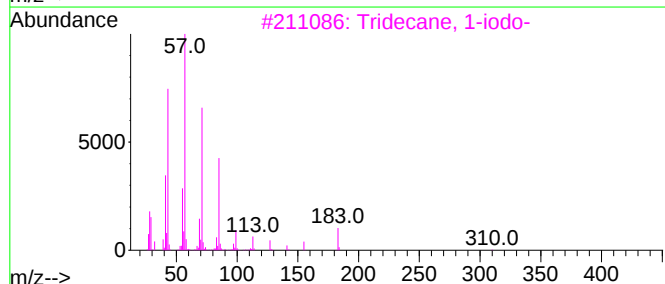
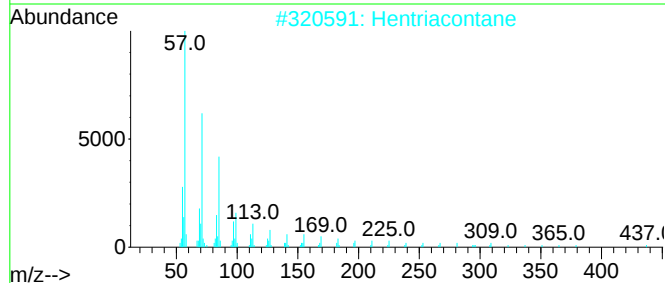
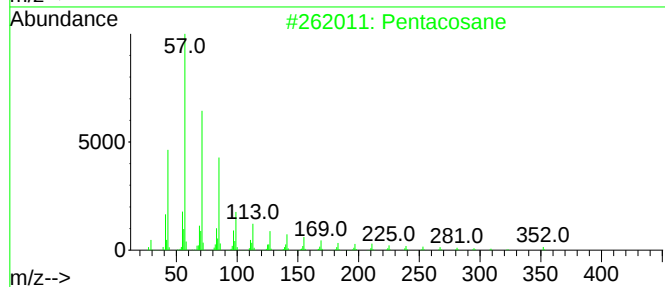
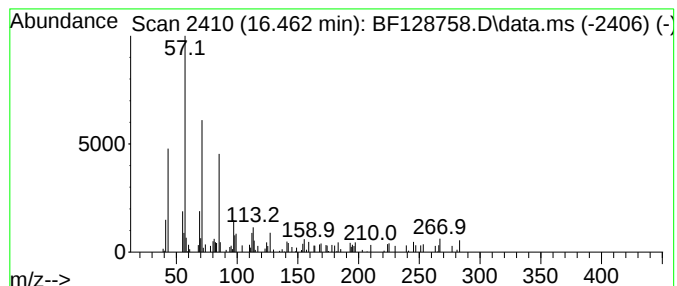
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.462	3.18 ng	69451	Perylene-d12	15.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	72
2			Hentriacontane	437	C31H64	000630-04-6	72
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4			Hexadecane	226	C16H34	000544-76-3	64
5			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061022\
Data File : BF128758.D
Acq On : 10 Jun 2022 14:50
Operator : CG\JU
Sample : N3287-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.004	2.1	ng	46124	1	6.798	441792	20.0
n-Hexadecanoic ...	11.851	6.8	ng	234003	4	11.327	685175	20.0
trans-Sinapalde...	12.004	2.2	ng	74118	4	11.327	685175	20.0
Octadecanoic acid	12.645	38.9	ng	1331540	4	11.327	685175	20.0
Tetracosane	13.321	3.7	ng	75084	5	13.974	409887	20.0
Triphenylphosph...	14.068	14.7	ng	302145	5	13.974	409887	20.0
Heptadecane, 9-...	14.557	7.4	ng	150998	5	13.974	409887	20.0
unknown14.933	14.933	5.4	ng	118680	6	15.433	436192	20.0
Octacosane	15.104	7.0	ng	153837	6	15.433	436192	20.0
Heneicosane	15.733	4.4	ng	96613	6	15.433	436192	20.0
.gamma.-Sitosterol	16.209	8.5	ng	184963	6	15.433	436192	20.0
Pentacosane	16.462	3.2	ng	69451	6	15.433	436192	20.0