

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063022\
 Data File : BF129066.D
 Acq On : 30 Jun 2022 18:58
 Operator : CG\JU
 Sample : N3450-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PH1-BOT-18

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129066.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.369	5	14	24	rVB	2633827	3491039	28.81%	4.055%
2	5.234	499	501	514	rVB	90548	124921	1.03%	0.145%
3	5.593	556	562	565	rBV	9127001	9538547	78.72%	11.080%
4	6.581	724	730	733	rBV	8388705	9765153	80.59%	11.344%
5	6.692	746	749	752	rBV	174690	122251	1.01%	0.142%
6	6.957	790	794	797	rVB	2846589	2417843	19.95%	2.809%
7	7.522	883	890	893	rBV	5963463	6578542	54.29%	7.642%
8	8.239	1007	1012	1015	rVB	3680975	3182939	26.27%	3.697%
9	9.316	1189	1195	1198	rBV	12109494	12117687	100.00%	14.076%
10	9.998	1305	1311	1314	rBV	4334572	3604126	29.74%	4.187%
11	10.792	1439	1446	1449	rBV	7903290	7676066	63.35%	8.917%
12	10.892	1459	1463	1465	rBV	160895	175088	1.44%	0.203%
13	11.492	1558	1565	1568	rBV	4160353	3680722	30.37%	4.276%
14	12.004	1648	1652	1661	rBV	845113	939960	7.76%	1.092%
15	12.792	1783	1786	1790	rBV	350257	340501	2.81%	0.396%
16	13.080	1830	1835	1839	rVB	11081280	11832095	97.64%	13.745%
17	14.016	1990	1994	2003	rBV2	374714	841455	6.94%	0.977%
18	14.139	2011	2015	2019	rVB	3358593	2798076	23.09%	3.250%
19	14.233	2026	2031	2036	rBV	503175	567782	4.69%	0.660%
20	14.998	2158	2161	2164	rBV	162981	151643	1.25%	0.176%
21	15.274	2205	2208	2216	rVB2	94819	122191	1.01%	0.142%
22	15.662	2269	2274	2284	rVB2	1821422	2326768	19.20%	2.703%
23	16.480	2405	2413	2430	rVB4	403649	1343773	11.09%	1.561%
24	16.627	2432	2438	2445	rBV	1135107	1896863	15.65%	2.203%
25	17.892	2647	2653	2662	rBV5	197780	449020	3.71%	0.522%

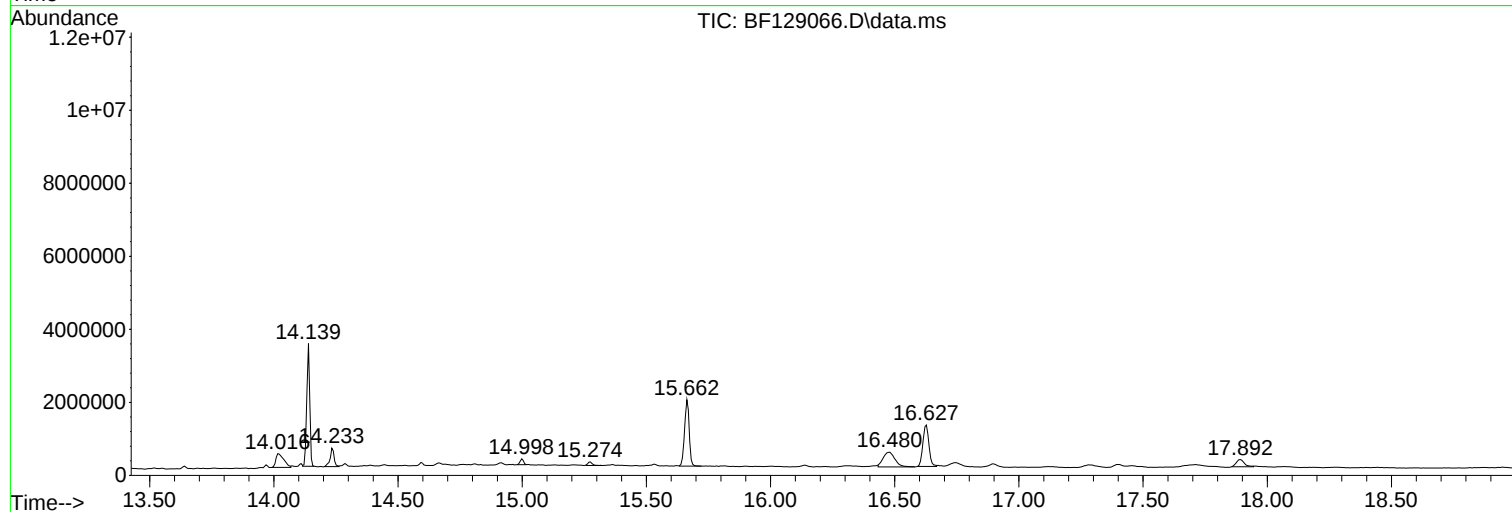
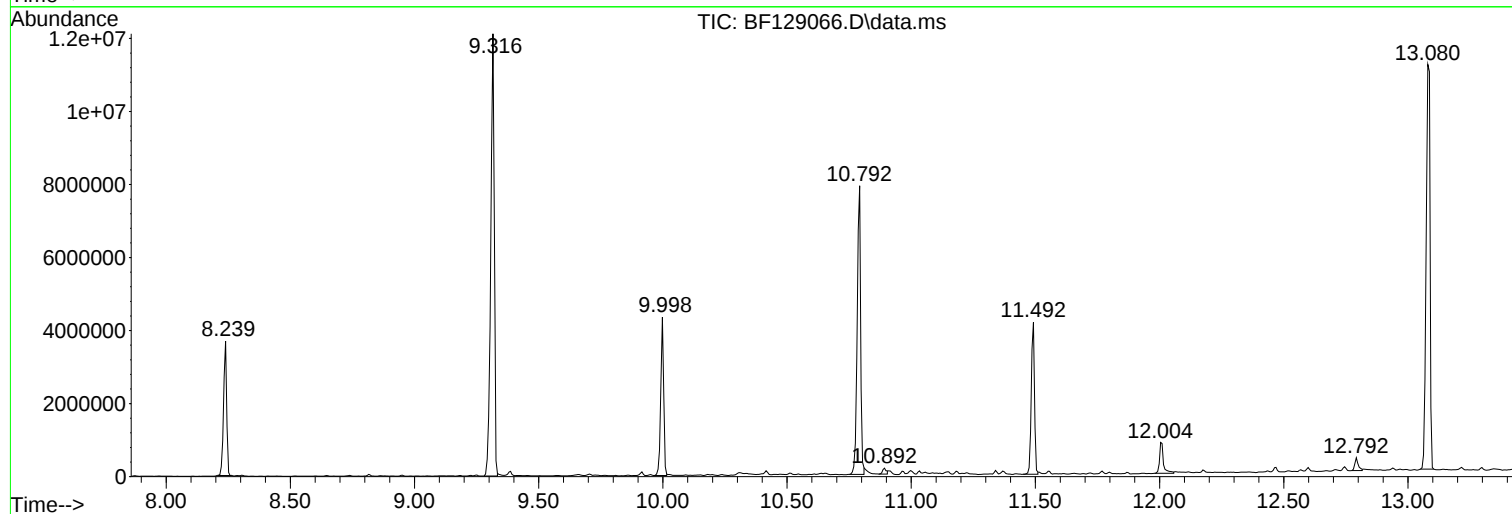
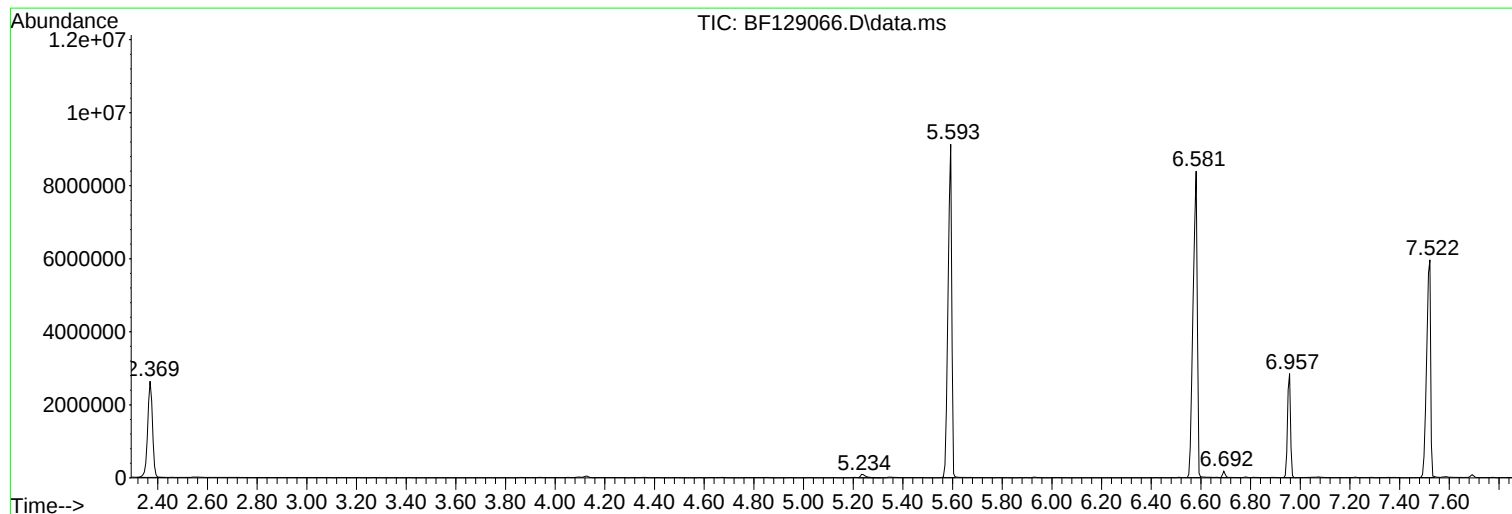
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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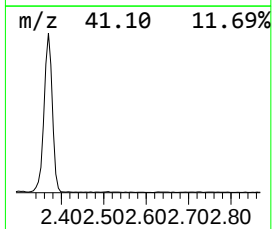
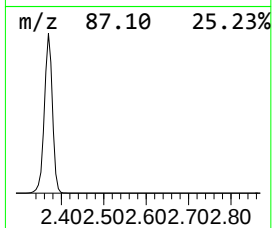
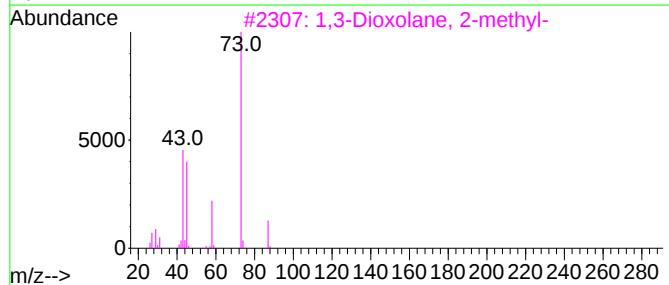
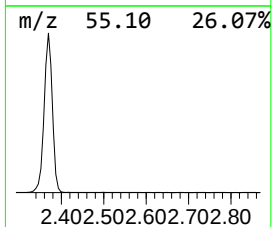
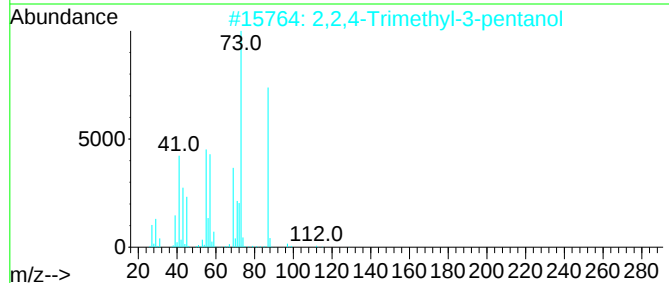
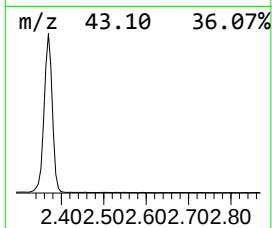
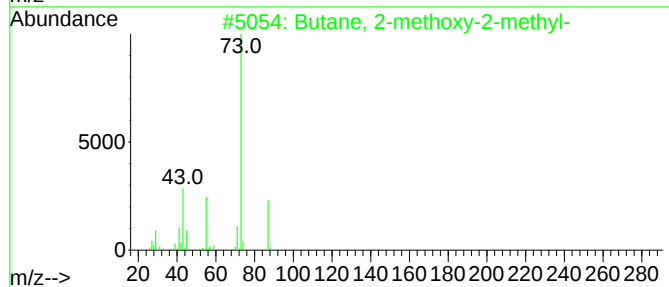
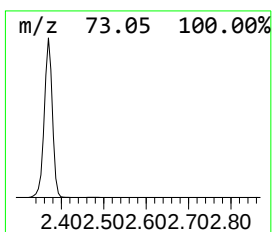
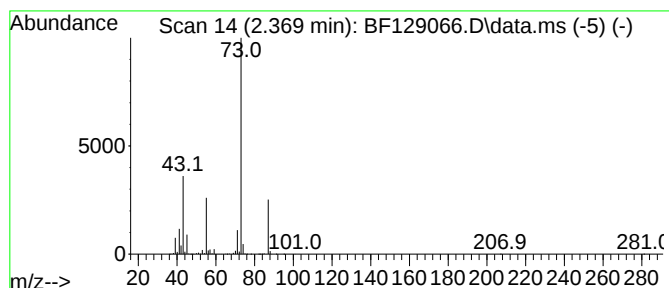
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.369	28.88 ng	3491040	1,4-Dichlorobenzene-d4	6.957

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	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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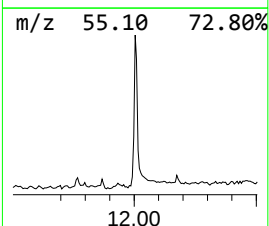
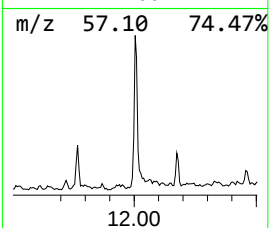
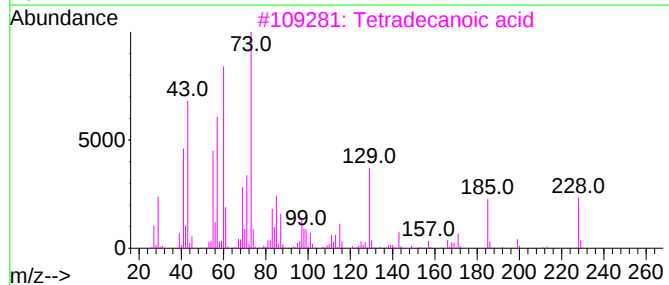
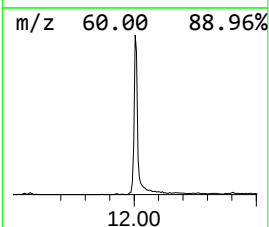
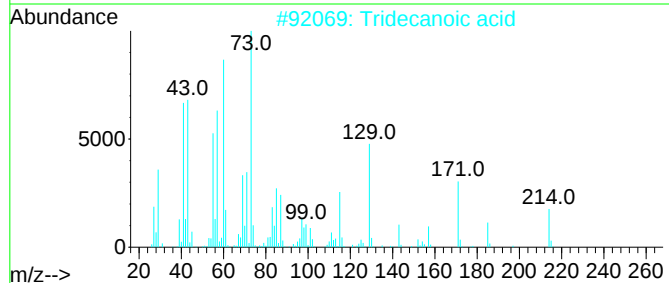
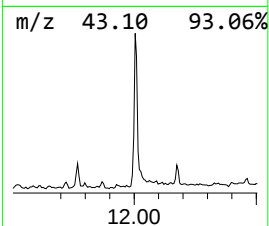
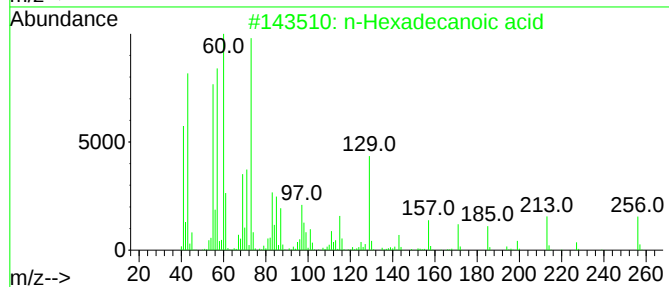
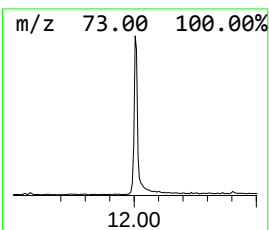
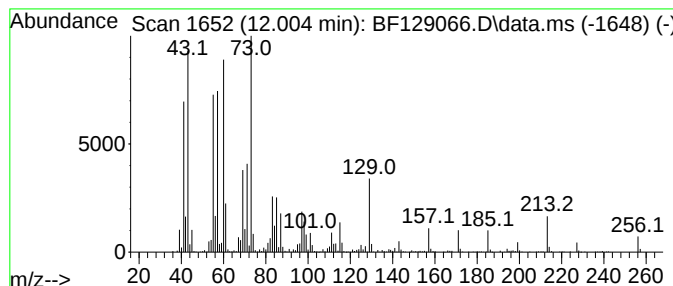
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.004	5.11 ng	939960	Phenanthrene-d10	11.492

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	94
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5		8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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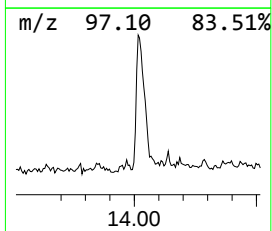
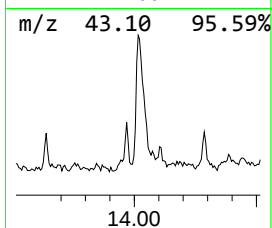
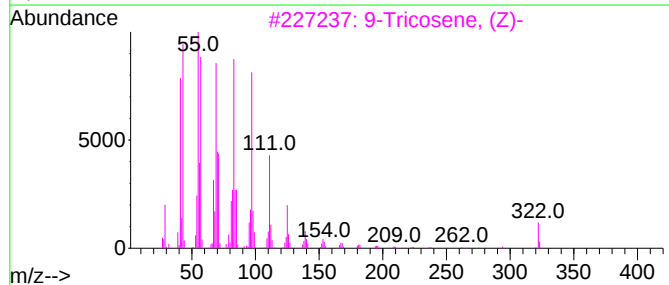
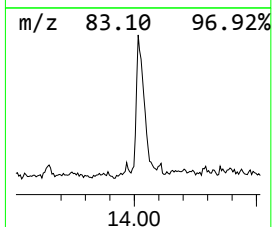
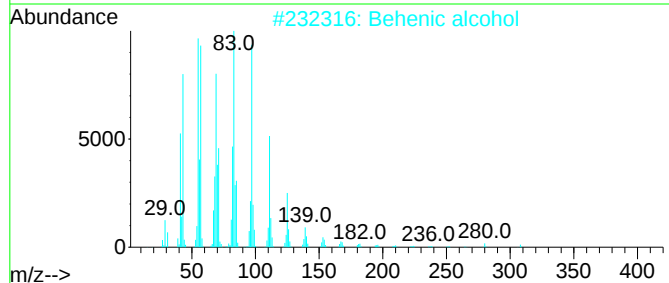
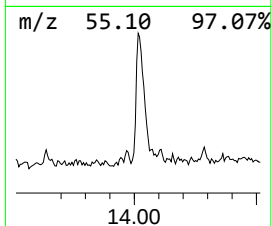
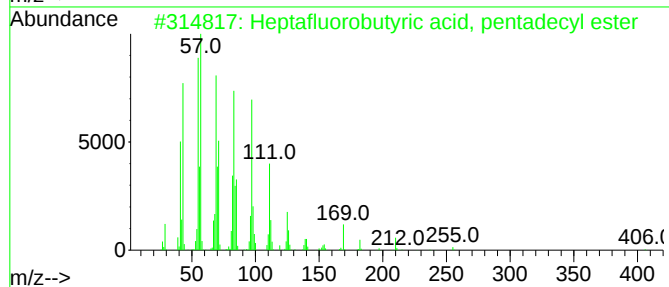
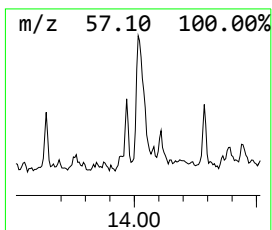
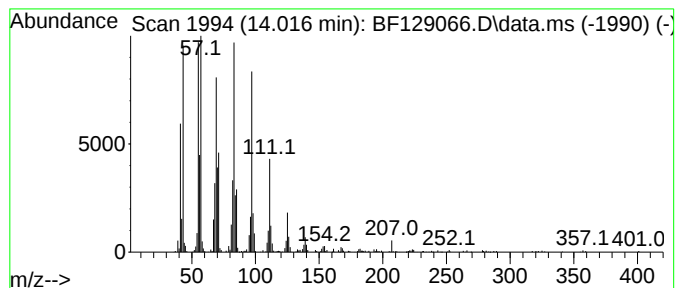
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.015	6.01 ng	841455	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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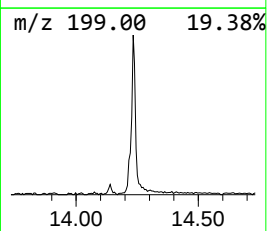
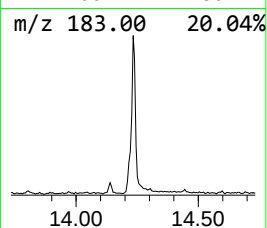
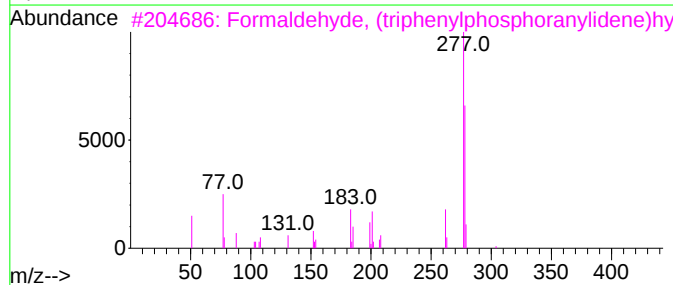
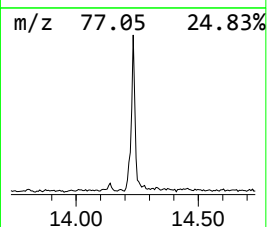
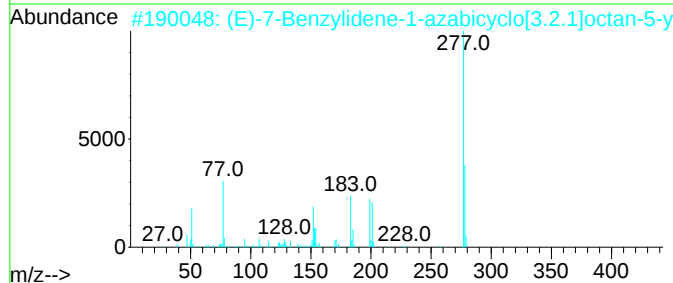
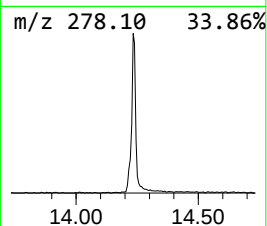
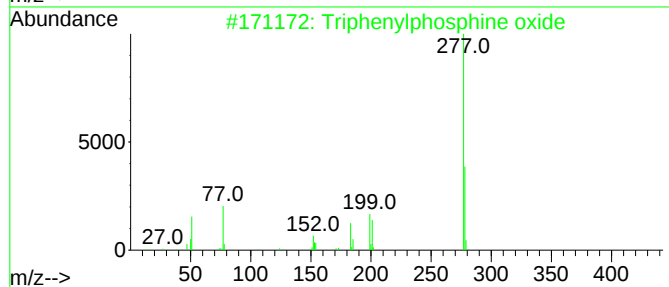
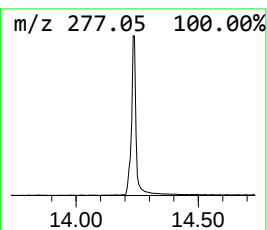
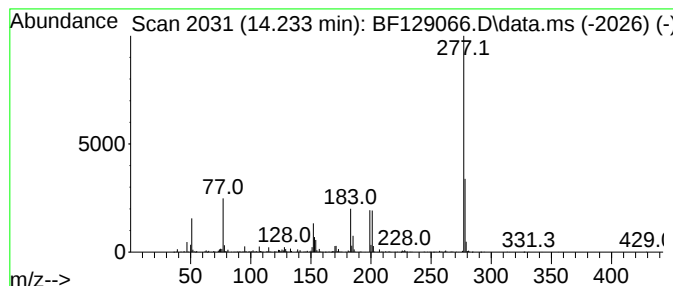
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.233	4.06 ng	567782	Chrysene-d12	14.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	76
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	50
4			1H-Indole-3-acetic acid, 5-[(tri...]	277	C14H19NO3Si	072101-35-0	17
5			4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	12



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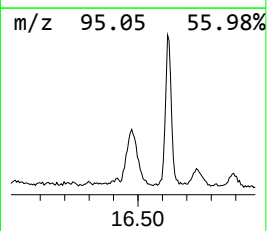
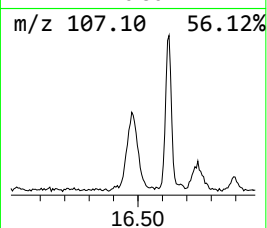
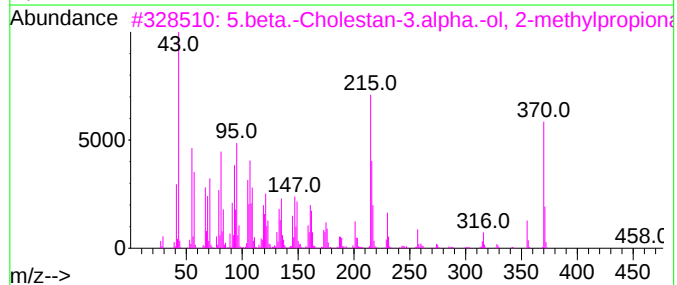
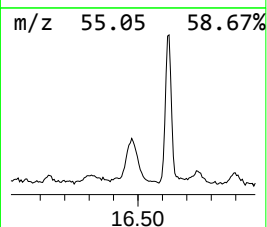
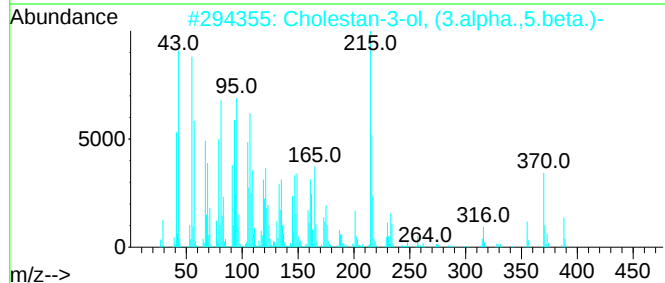
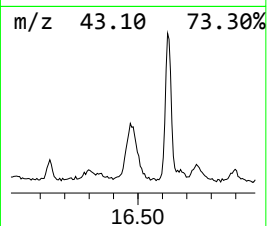
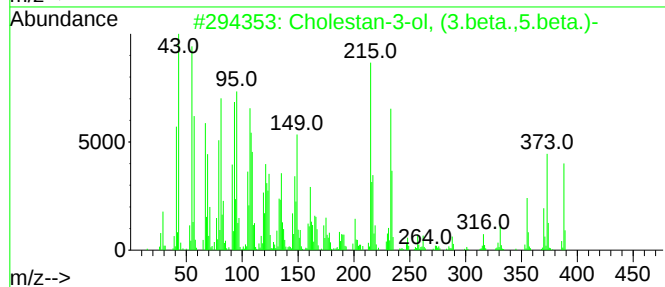
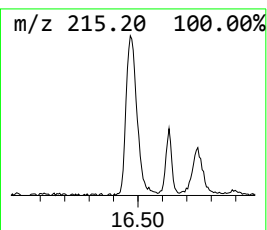
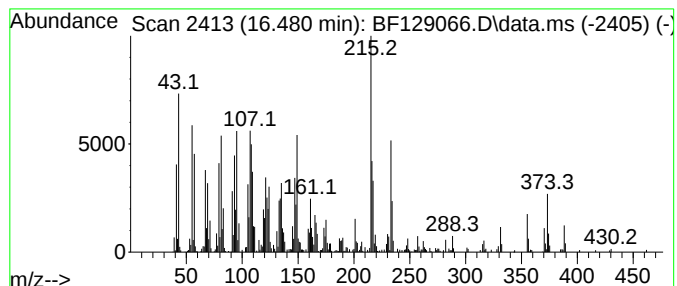
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	11.55 ng	1343770	Perylene-d12	15.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	97
2			Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	83
3			5.beta.-Cholestan-3.alpha.-ol, 2...	458	C31H54O2	1000514-95-7	64
4			Cholestanol	388	C27H48O	000080-97-7	46
5			Cholestan-3-ol	388	C27H48O	027409-41-2	46



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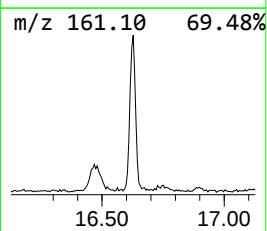
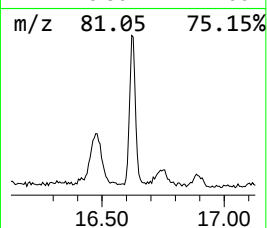
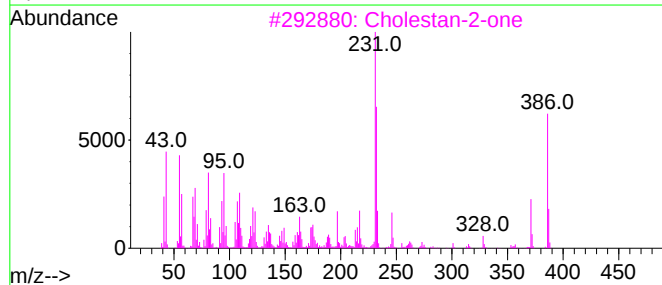
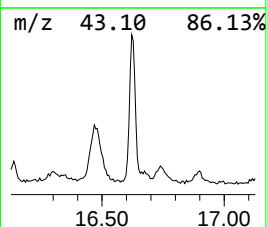
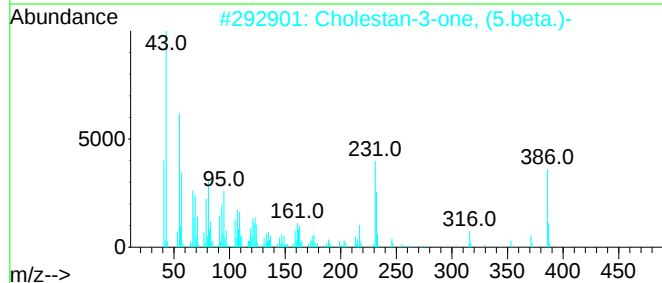
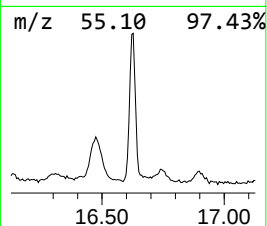
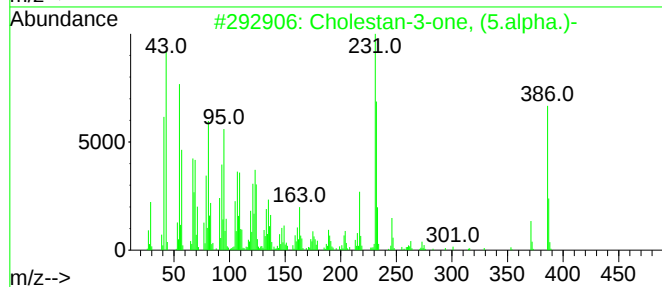
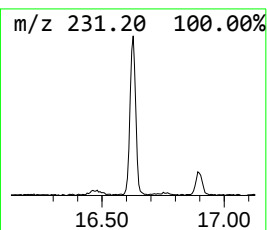
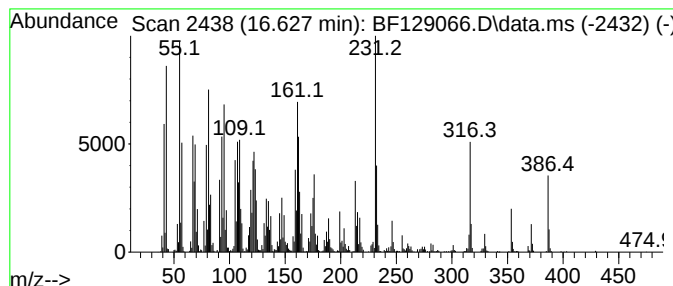
Instrument :
BNA_F
ClientSampleId :
PH1-BOT-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cholestan-3-one, (5.alpha.)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.627	16.30 ng	1896860	Perylene-d12		15.663	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cholestan-3-one, (5.alpha.)-		386	C27H46O	000566-88-1	93
2	Cholestan-3-one, (5.beta.)-		386	C27H46O	000601-53-6	44
3	Cholestan-2-one		386	C27H46O	1010210-43-4	41
4	Cholestan-3-one		386	C27H46O	015600-08-5	35
5	2-Iodo-2'-methoxybenzanilide		353	C14H12INO2	036684-47-6	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063022\
Data File : BF129066.D
Acq On : 30 Jun 2022 18:58
Operator : CG\JU
Sample : N3450-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH1-BOT-18

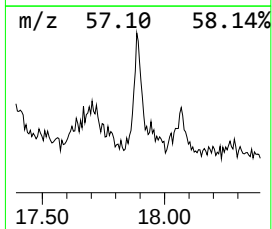
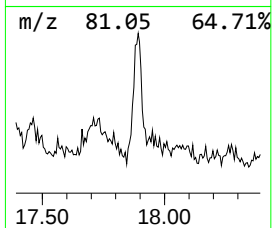
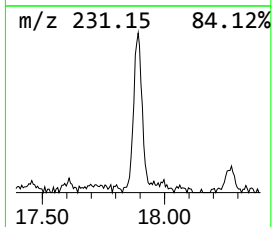
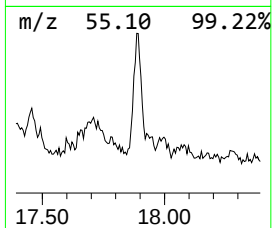
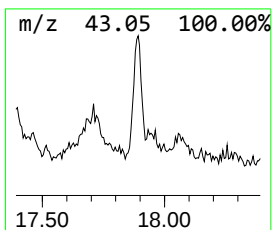
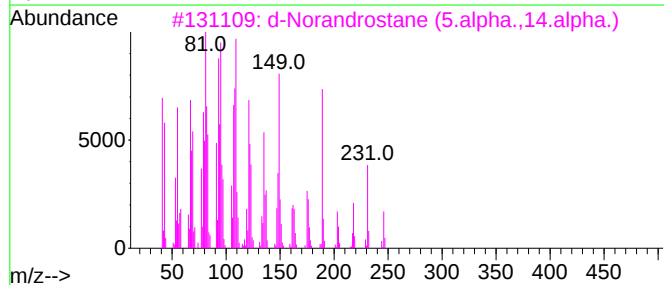
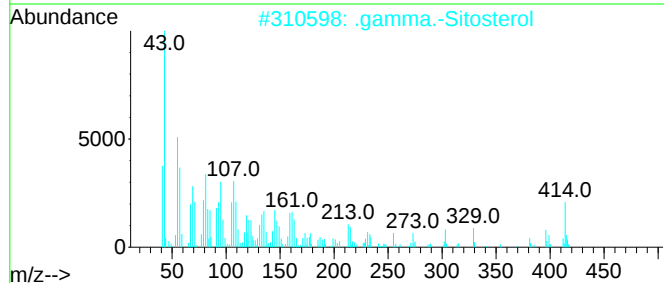
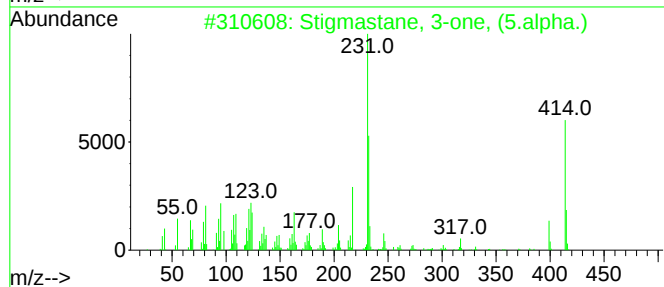
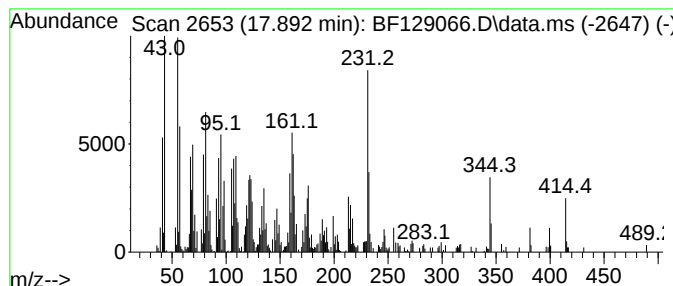
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown17.892 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	3.86 ng	449020	Perylene-d12	15.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Stigmastane, 3-one, (5.alpha.)	414	C29H50O	1000437-00-8	45
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	41
3			d-Norandrostane (5.alpha.,14.alp...	246	C18H30	1000281-13-8	27
4			Coprost-25-en-16,22-epoxy-3.alph...	400	C27H44O2	122337-93-3	25
5			Cholestan-3-one, 4,4-dimethyl-, ...	414	C29H50O	002097-85-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF063022\
Data File : BF129066.D
Acq On : 30 Jun 2022 18:58
Operator : CG\JU
Sample : N3450-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PH1-BOT-18

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062922.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...	2.369	28.9	ng	3491040	1	6.957	2417840	20.0
n-Hexadecanoic ...	12.004	5.1	ng	939960	4	11.492	3680720	20.0
Heptafluorobuty...	14.015	6.0	ng	841455	5	14.139	2798080	20.0
Triphenylphosph...	14.233	4.1	ng	567782	5	14.139	2798080	20.0
Cholestan-3-ol,...	16.480	11.6	ng	1343770	6	15.663	2326770	20.0
Cholestan-3-one...	16.627	16.3	ng	1896860	6	15.663	2326770	20.0
unknown17.892	17.892	3.9	ng	449020	6	15.663	2326770	20.0