

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128541.D
 Acq On : 28 May 2022 11:32
 Operator : CG\JU
 Sample : N2930-11
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P005-SS003-2430-01

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: BF128541.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.375	173	185	198	rBV	290100	837685	15.21%	2.093%
2	5.075	471	474	480	rVB	56057	70623	1.28%	0.176%
3	5.457	533	539	542	rBV	4226075	4425333	80.33%	11.056%
4	6.463	704	710	713	rBV	3868879	4580911	83.15%	11.445%
5	6.834	770	773	777	rVB	1295403	1159951	21.06%	2.898%
6	7.398	864	869	872	rBV	3101746	3111623	56.48%	7.774%
7	8.116	987	991	995	rBV	1681006	1557126	28.26%	3.890%
8	9.198	1169	1175	1178	rBV	5449672	5424036	98.46%	13.551%
9	9.310	1191	1194	1198	rVB	97008	88008	1.60%	0.220%
10	9.875	1285	1290	1294	rBV	2070399	1831764	33.25%	4.576%
11	10.663	1418	1424	1428	rBV	3514941	3602073	65.38%	8.999%
12	11.363	1539	1543	1546	rBV	2278217	1909656	34.66%	4.771%
13	11.428	1549	1554	1557	rVB2	70832	66159	1.20%	0.165%
14	11.892	1628	1633	1648	rBV	478584	513559	9.32%	1.283%
15	12.169	1675	1680	1685	rBV	45135	58686	1.07%	0.147%
16	12.680	1763	1767	1780	rBV	152035	192562	3.50%	0.481%
17	12.957	1809	1814	1817	rBV	5610425	5509064	100.00%	13.764%
18	13.863	1964	1968	1969	rBV	70520	79087	1.44%	0.198%
19	13.898	1969	1974	1987	rVB3	203543	600496	10.90%	1.500%
20	14.004	1987	1992	1995	rBV	1804755	1652246	29.99%	4.128%
21	14.098	2003	2008	2017	rVB	416167	462068	8.39%	1.154%
22	14.174	2018	2021	2026	rVB	68108	61747	1.12%	0.154%
23	14.480	2070	2073	2077	rBV	68236	60692	1.10%	0.152%
24	15.133	2179	2184	2188	rBV	65131	74507	1.35%	0.186%
25	15.186	2189	2193	2198	rBV	219952	268680	4.88%	0.671%
26	15.468	2235	2241	2246	rBV2	1110841	1355206	24.60%	3.386%
27	15.733	2276	2286	2292	rBV4	85459	226825	4.12%	0.567%
28	15.957	2319	2324	2330	rBV	40363	63471	1.15%	0.159%
29	16.098	2341	2348	2359	rBV	35395	117138	2.13%	0.293%
30	16.339	2385	2389	2395	rVB	44324	65253	1.18%	0.163%

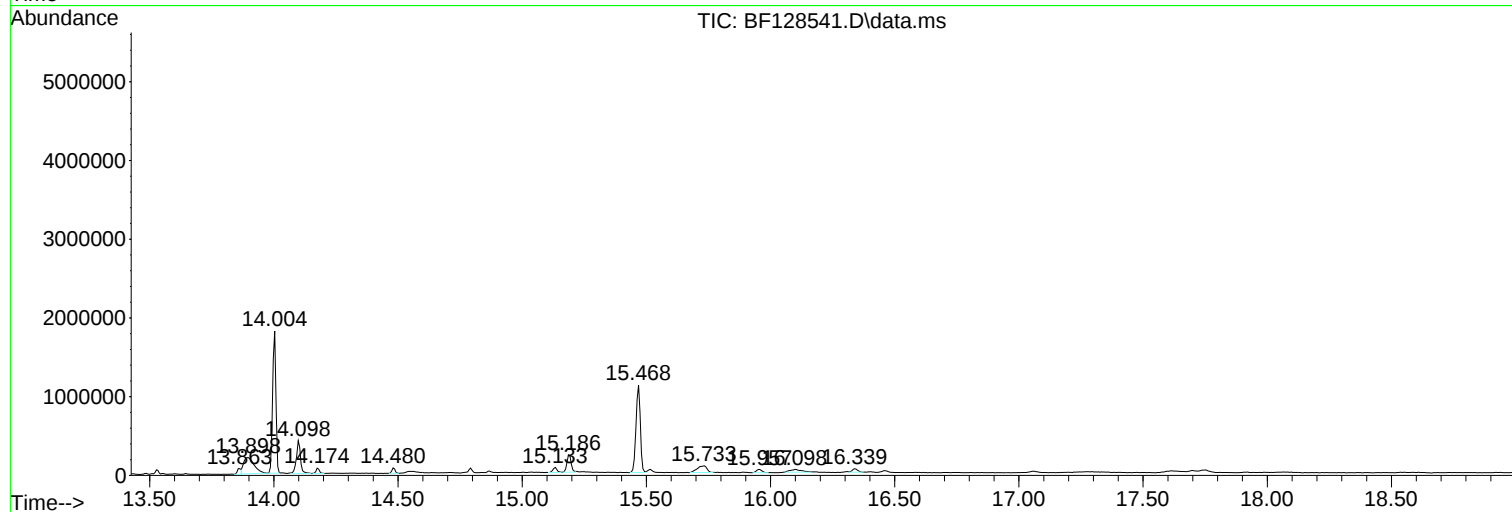
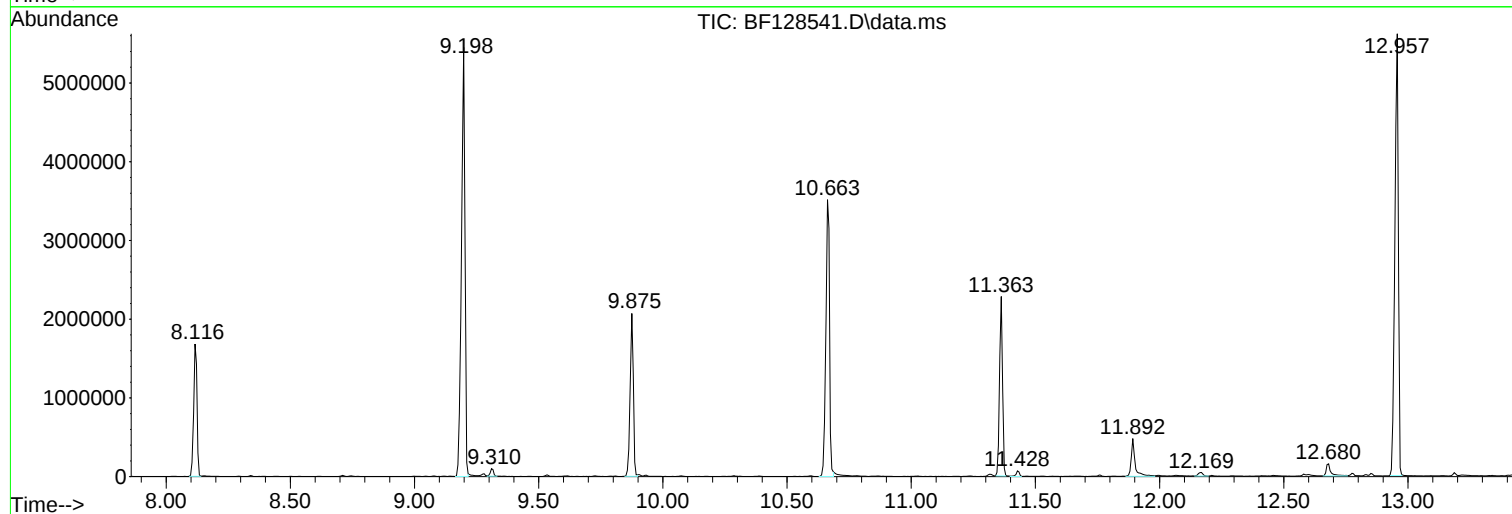
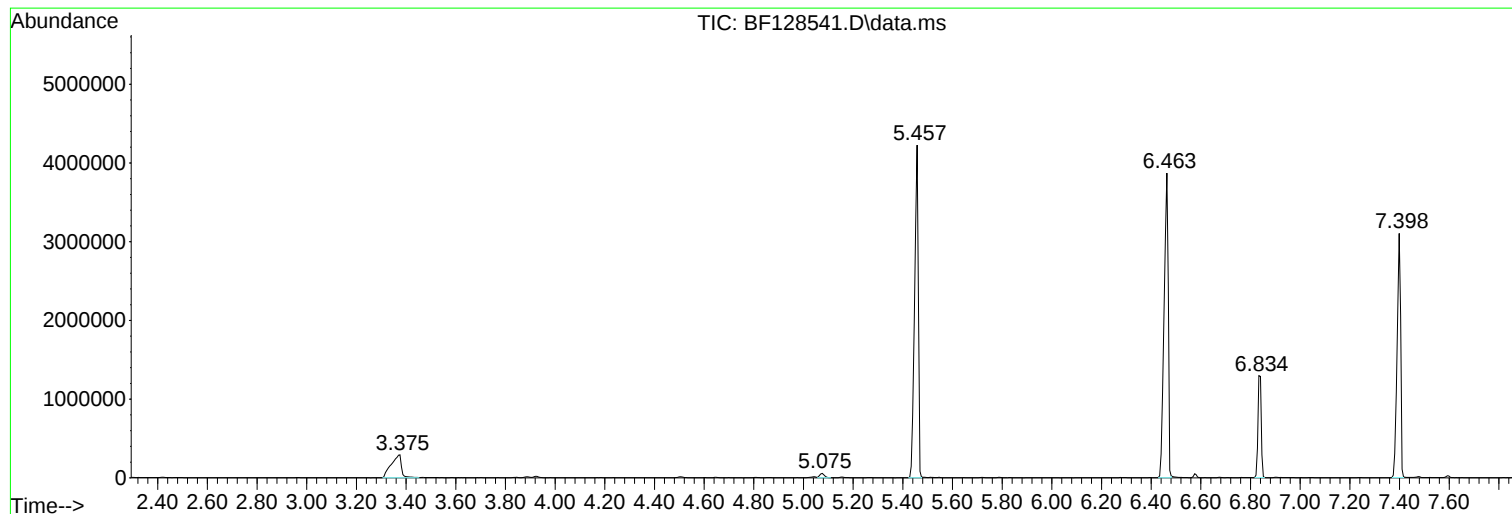
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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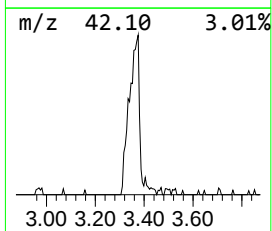
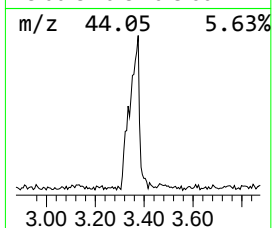
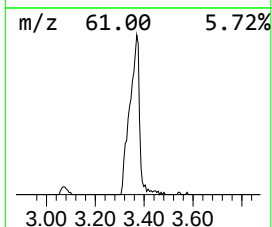
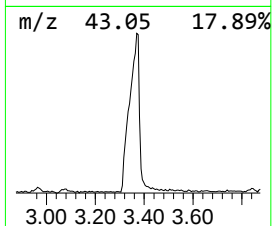
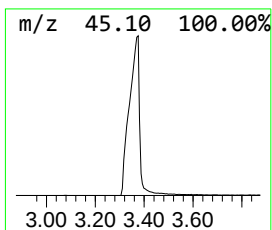
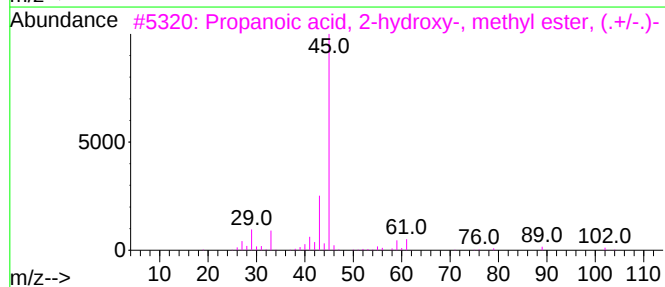
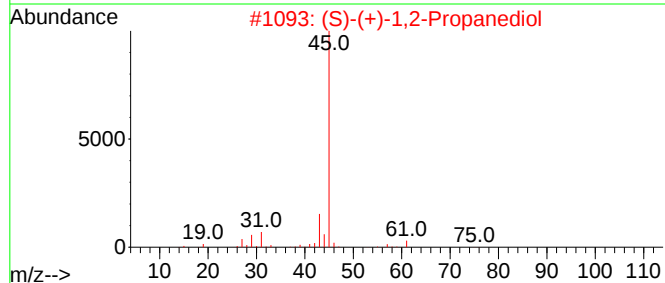
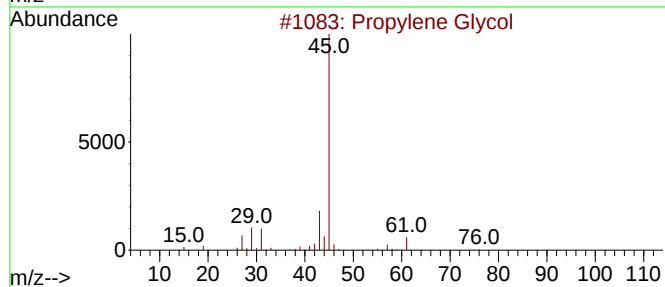
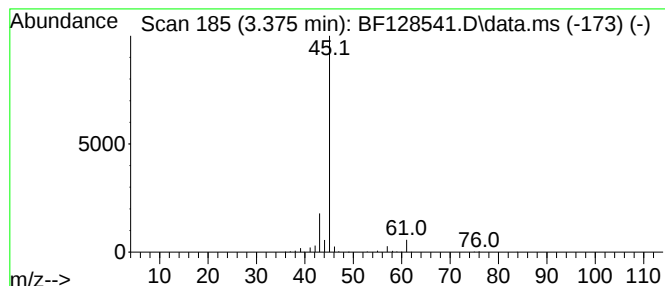
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	14.44 ng	837685	1,4-Dichlorobenzene-d4	6.840

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			2-Butanol	74	C4H10O	000078-92-2	9



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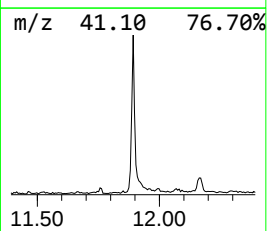
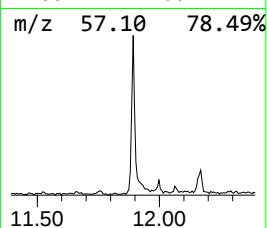
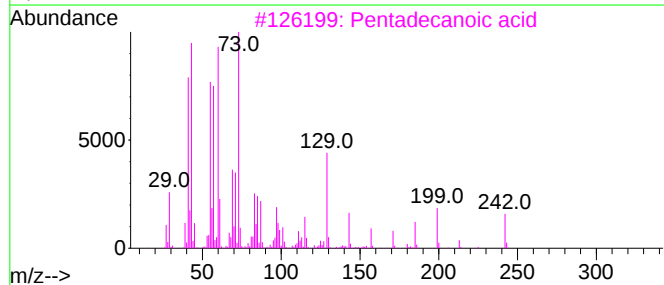
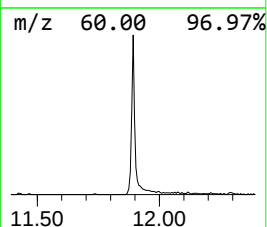
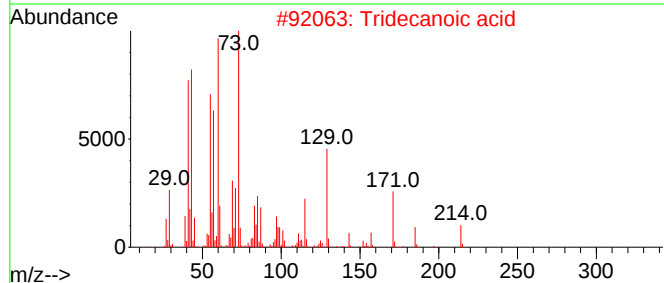
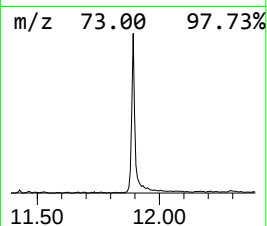
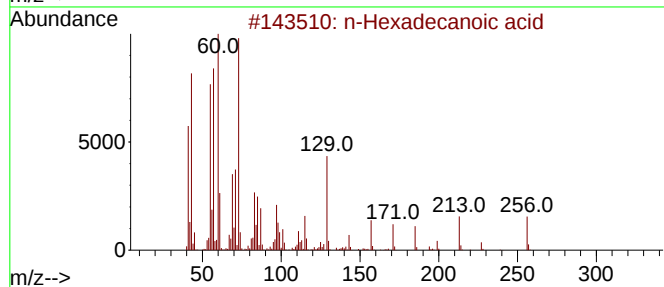
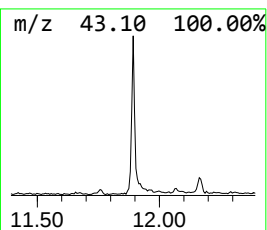
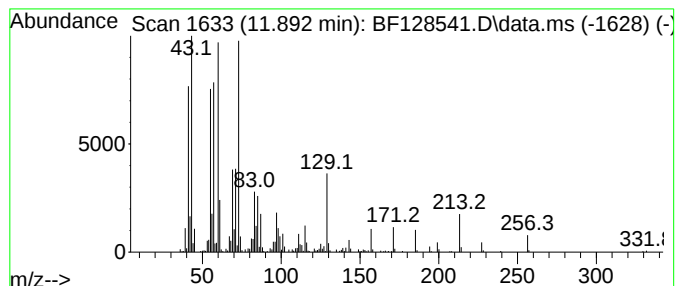
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	5.38 ng	513559	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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	72



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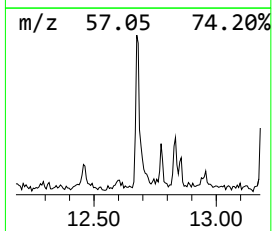
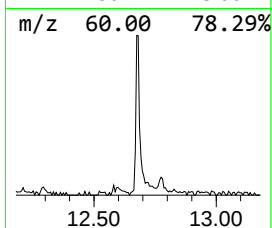
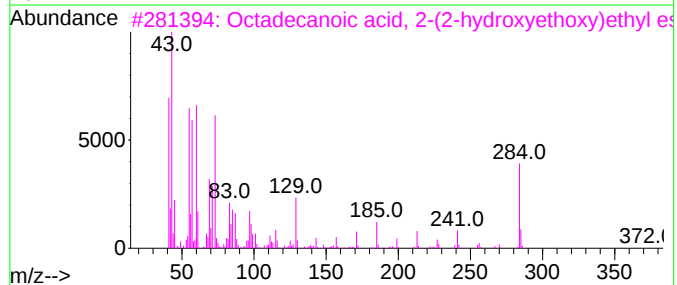
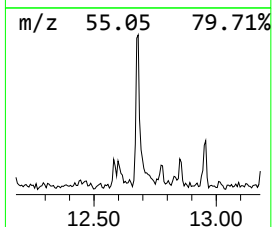
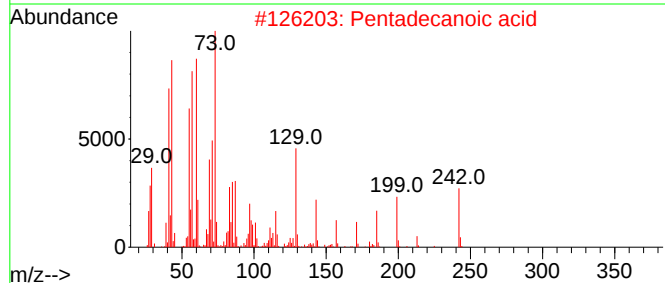
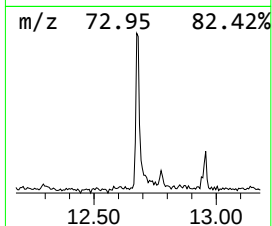
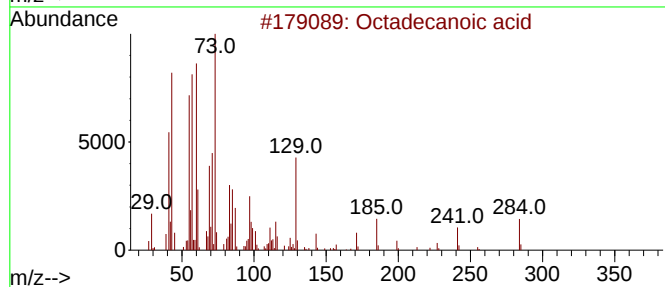
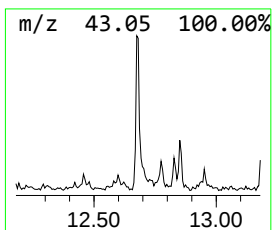
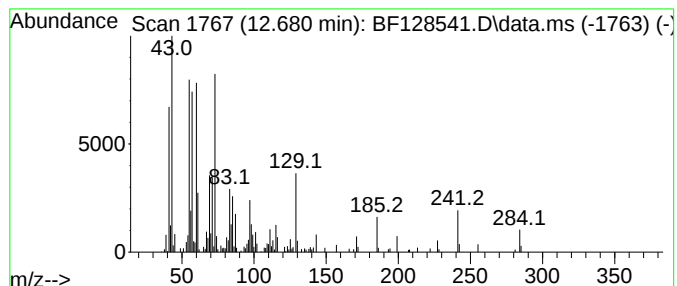
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.02 ng	192562	Phenanthrene-d10	11.363

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	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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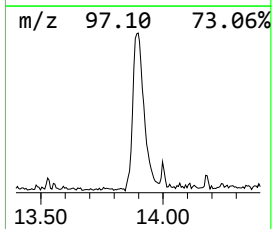
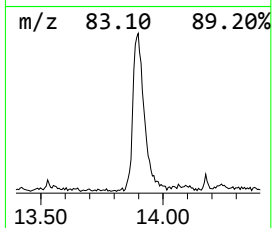
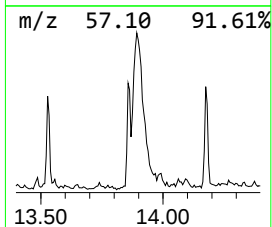
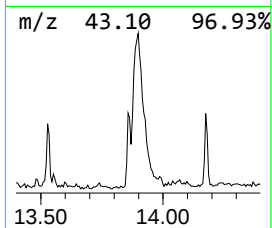
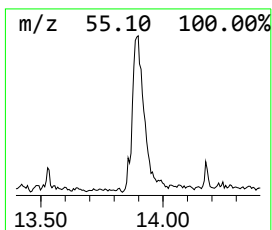
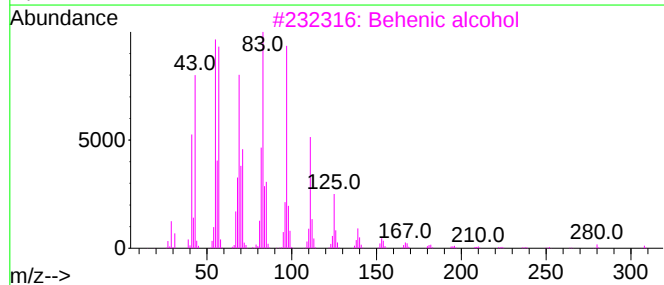
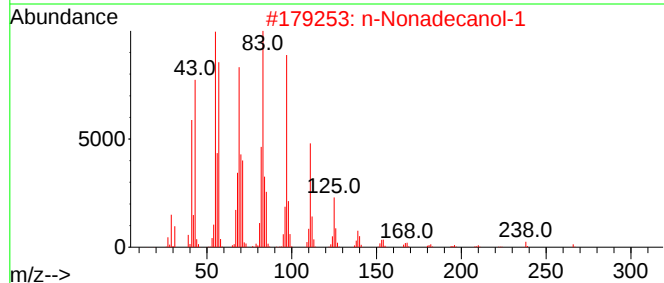
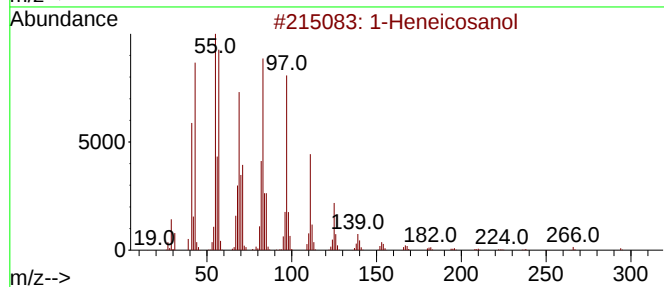
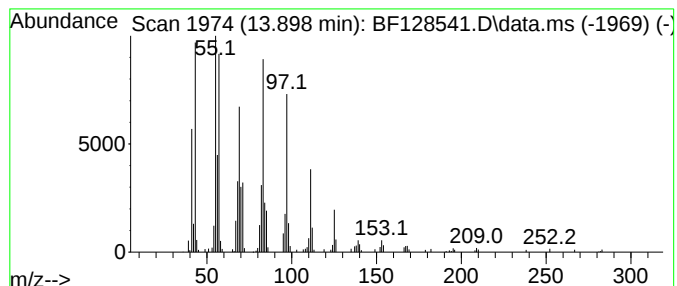
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Peak Number 4 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	7.27 ng	600496	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			1-Octadecanol	270	C18H38O	000112-92-5	83
5			1-Tetracosene	336	C24H48	010192-32-2	81



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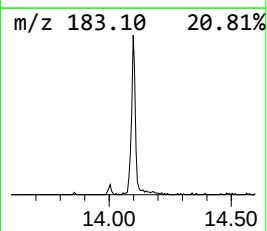
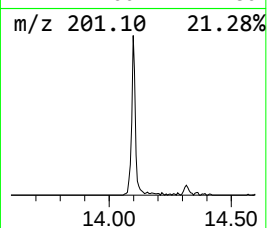
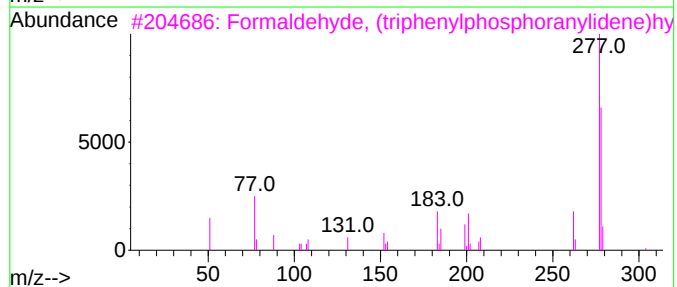
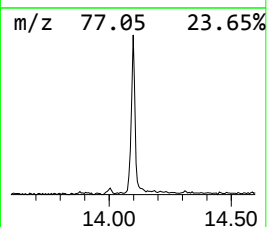
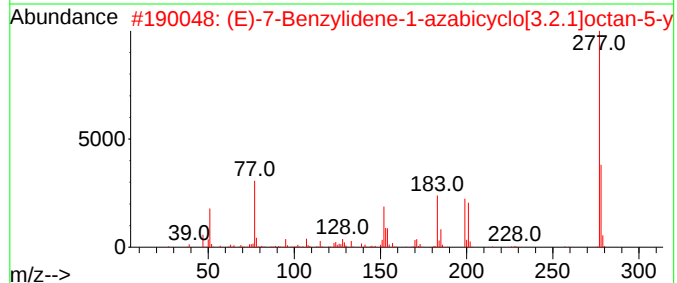
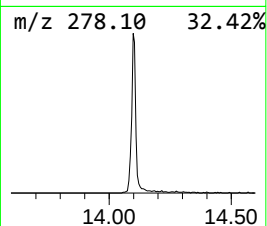
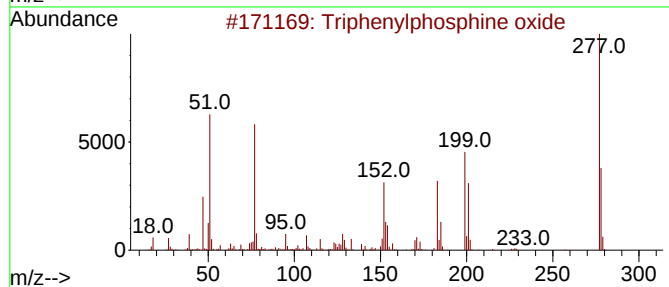
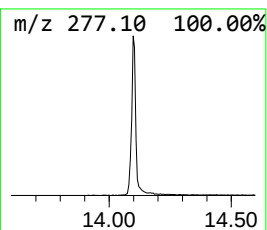
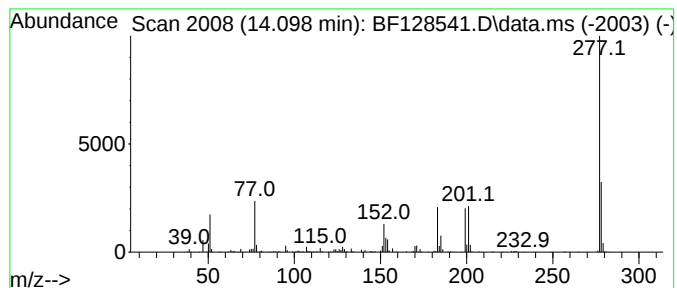
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	5.59 ng	462068	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	96
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19NO3S	1000483-83-4	91
3			Formaldehyde, (triphenylphosphor...]	304	C19H17N2P	015990-54-2	64
4			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	23



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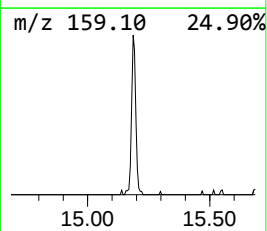
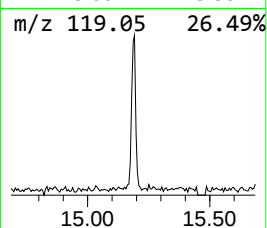
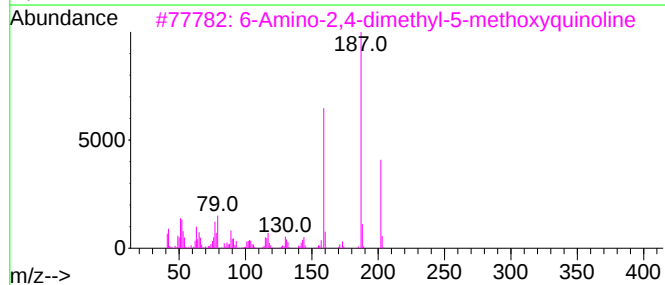
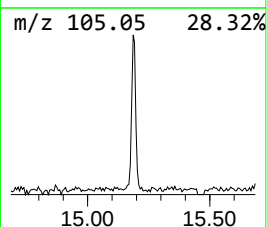
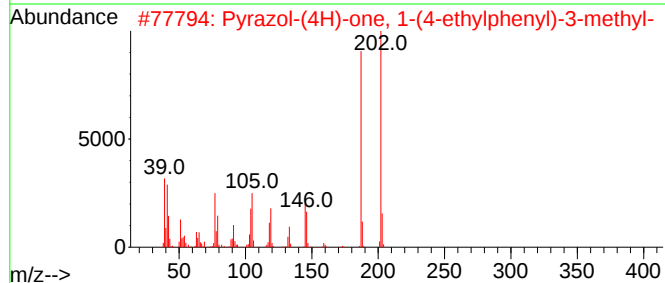
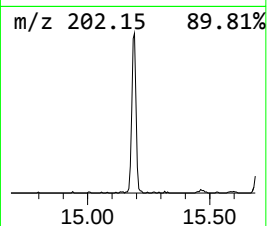
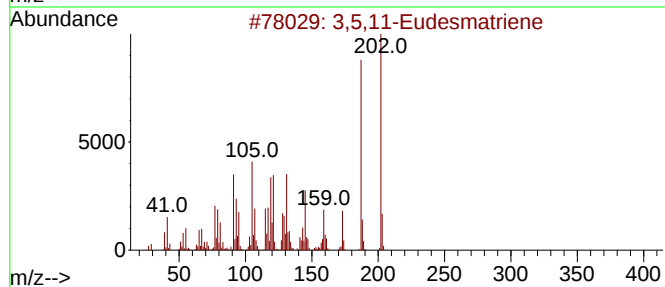
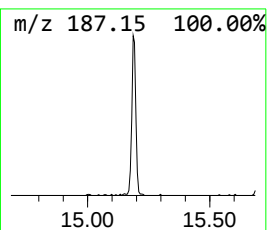
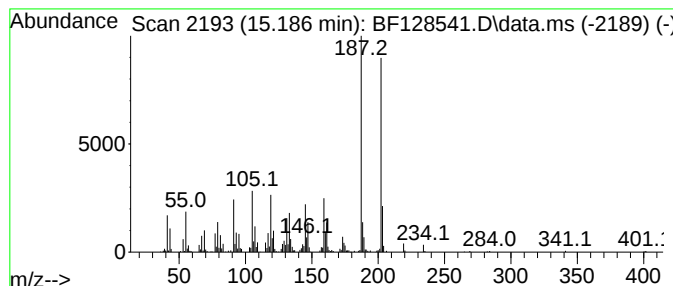
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 3,5,11-Eudesmatriene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	3.97 ng	268680	Perylene-d12	15.469

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,5,11-Eudesmatriene	202	C15H22	193615-07-5	64
2			Pyrazol-(4H)-one, 1-(4-ethylphen...	202	C12H14N2O	107430-31-9	59
3			6-Amino-2,4-dimethyl-5-methoxyqu...	202	C12H14N2O	084264-47-1	58
4			1,2-Dihydroharmaline	202	C12H14N2O	1010128-31-3	52
5			Quinoxaline, 2-tert-butyl-, 4-oxide	202	C12H14N2O	016007-51-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128541.D
Acq On : 28 May 2022 11:32
Operator : CG\JU
Sample : N2930-11
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P005-SS003-2430-01

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
Propylene Glycol	3.375	14.4	ng	837685	1	6.840	1159950	20.0
n-Hexadecanoic ...	11.892	5.4	ng	513559	4	11.363	1909660	20.0
Octadecanoic acid	12.680	2.0	ng	192562	4	11.363	1909660	20.0
1-Heneicosanol	13.898	7.3	ng	600496	5	14.004	1652250	20.0
Triphenylphosph...	14.098	5.6	ng	462068	5	14.004	1652250	20.0
3,5,11-Eudesmat...	15.186	4.0	ng	268680	6	15.469	1355210	20.0
Cyclohexane, 3,...	15.733	3.4	ng	226825	6	15.469	1355210	20.0