

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
 Data File : BF128554.D
 Acq On : 28 May 2022 18:07
 Operator : CG\JU
 Sample : N2933-13
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P023-SS003-0006-01

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: BF128554.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.346	178	180	197	rBV	26347	64717	1.21%	0.180%
2	5.081	471	475	481	rVB	64261	86716	1.62%	0.241%
3	5.457	534	539	542	rBV	3984571	4495808	84.05%	12.505%
4	6.463	704	710	713	rBV	3851958	4656587	87.06%	12.953%
5	6.575	726	729	734	rVB	91105	67215	1.26%	0.187%
6	6.834	770	773	777	rBV	1167175	1020528	19.08%	2.839%
7	7.398	864	869	872	rBV	2960653	3185634	59.56%	8.861%
8	8.116	987	991	995	rBV	1438112	1339437	25.04%	3.726%
9	9.198	1169	1175	1178	rBV	5523920	5348883	100.00%	14.878%
10	9.875	1284	1290	1293	rBV	1861011	1520338	28.42%	4.229%
11	10.663	1419	1424	1428	rBV	3467843	3470815	64.89%	9.654%
12	11.363	1539	1543	1546	rVB	1814523	1491680	27.89%	4.149%
13	11.757	1607	1610	1614	rVB	109633	92022	1.72%	0.256%
14	11.892	1629	1633	1643	rBV	443979	425040	7.95%	1.182%
15	12.469	1724	1731	1734	rBV	374726	361279	6.75%	1.005%
16	12.557	1743	1746	1748	rBV	76448	68764	1.29%	0.191%
17	12.616	1751	1756	1759	rVV	92161	100190	1.87%	0.279%
18	12.674	1763	1766	1779	rBV2	163524	196887	3.68%	0.548%
19	12.951	1808	1813	1817	rBV	4416779	4601713	86.03%	12.800%
20	13.321	1873	1876	1880	rBV	65433	57640	1.08%	0.160%
21	13.527	1907	1911	1917	rBV2	55235	79122	1.48%	0.220%
22	13.857	1965	1967	1970	rBV	48456	54743	1.02%	0.152%
23	13.910	1970	1976	1986	rVB3	83266	221742	4.15%	0.617%
24	13.998	1987	1991	1995	rBV	1098175	1058767	19.79%	2.945%
25	14.098	2002	2008	2016	rBV	480920	522093	9.76%	1.452%
26	14.868	2135	2139	2142	rVB	54808	57107	1.07%	0.159%
27	15.133	2180	2184	2188	rBV	55524	61172	1.14%	0.170%
28	15.468	2235	2241	2245	rBV	726629	908144	16.98%	2.526%
29	15.515	2245	2249	2254	rVB2	38677	58607	1.10%	0.163%
30	15.951	2319	2323	2328	rVB2	50679	72002	1.35%	0.200%
31	16.462	2405	2410	2419	rVB2	35544	75763	1.42%	0.211%
32	17.286	2544	2550	2558	rVB5	62621	129552	2.42%	0.360%

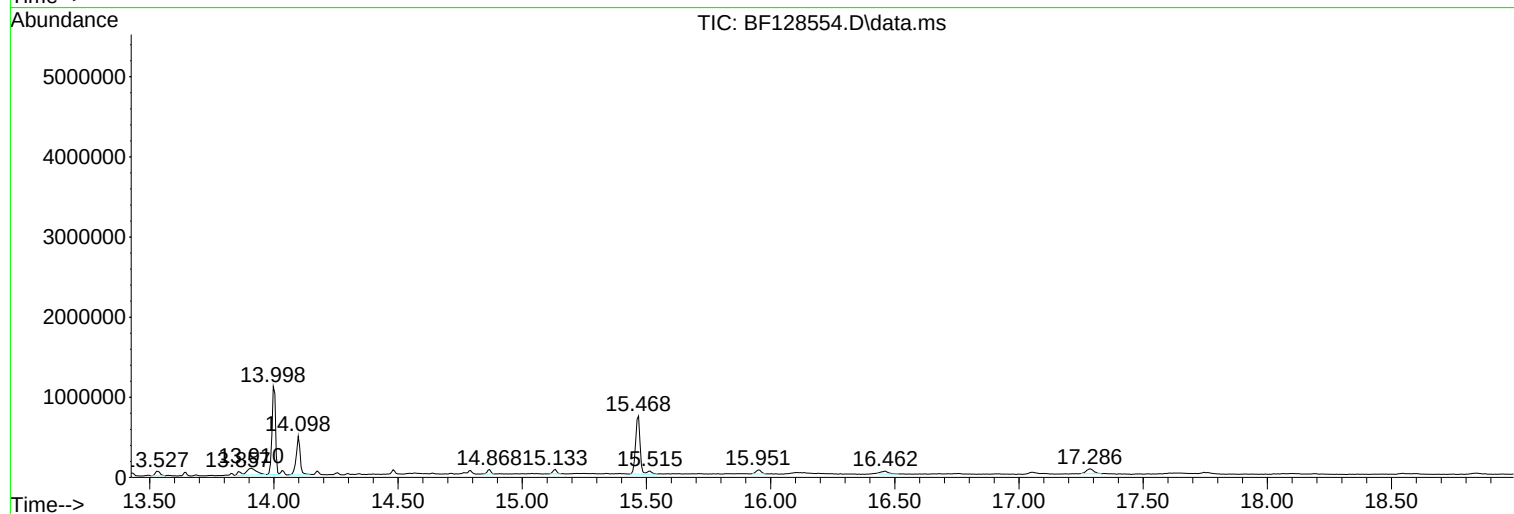
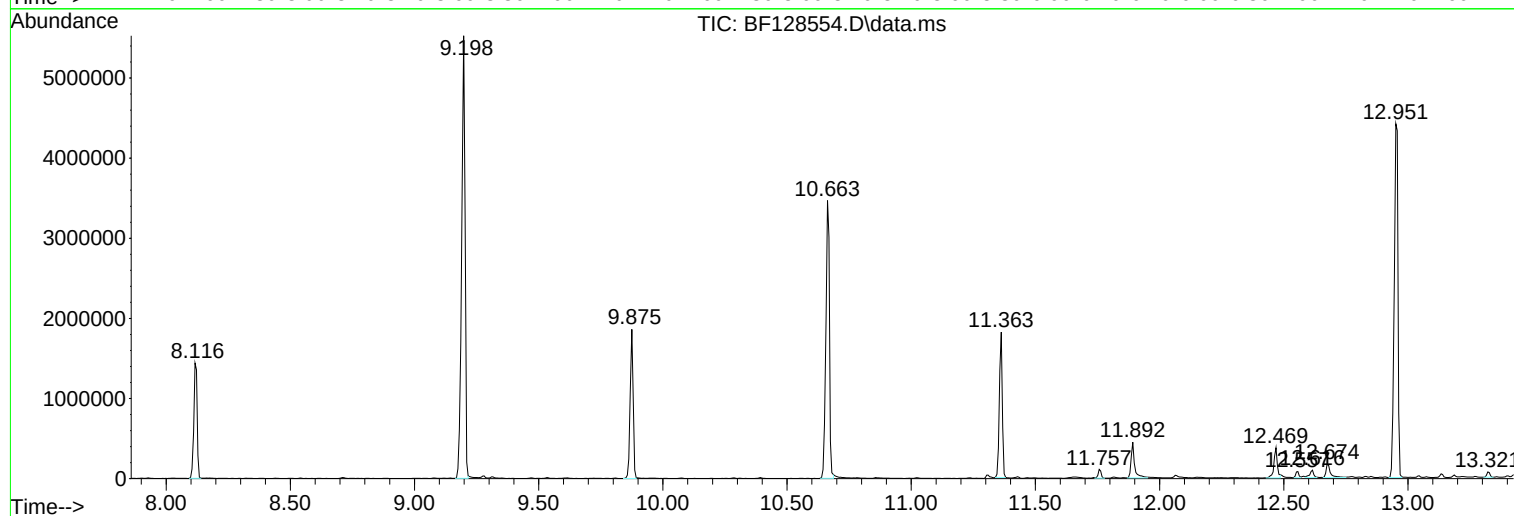
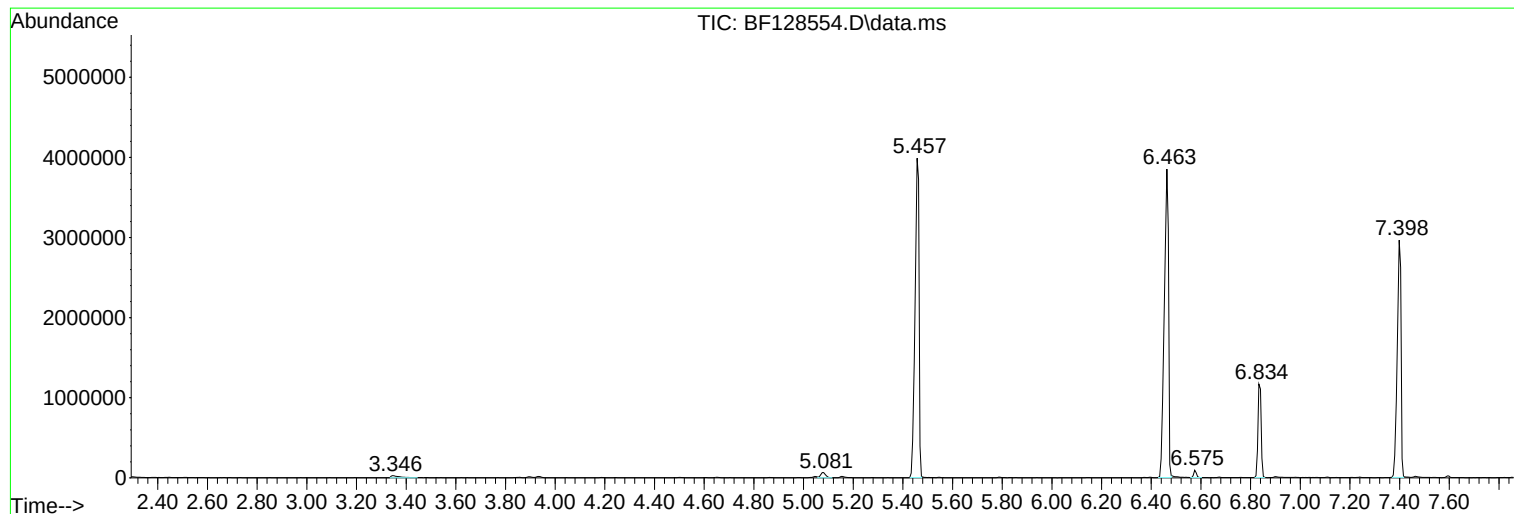
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF052622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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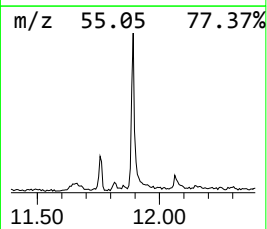
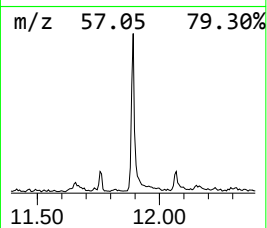
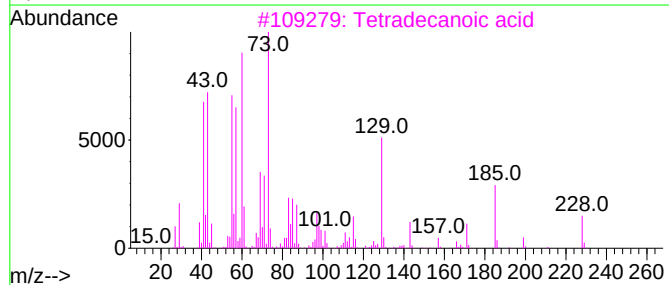
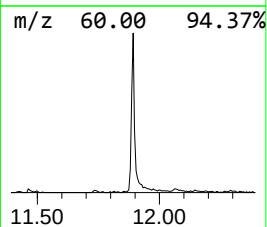
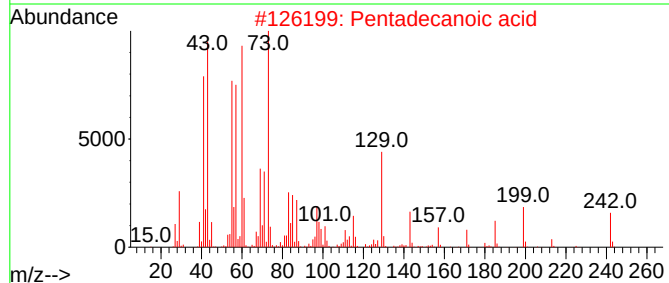
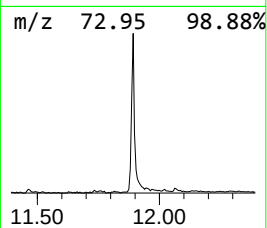
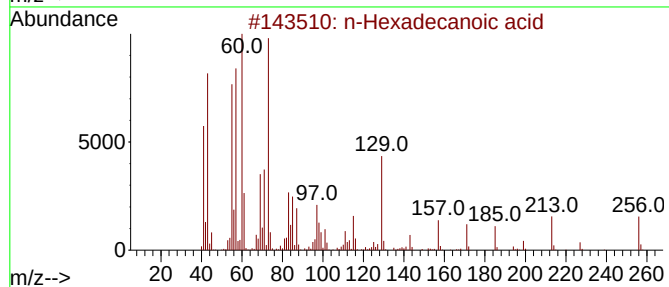
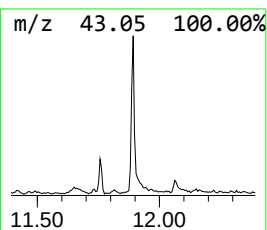
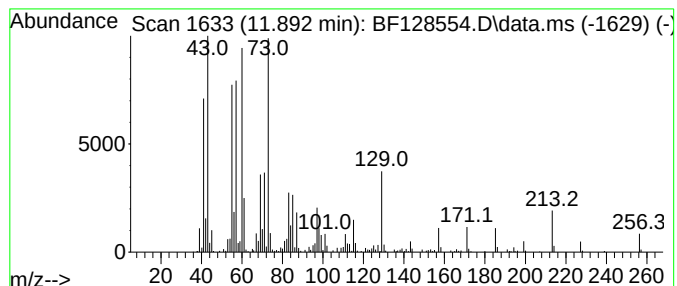
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	5.70 ng	425040	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	52



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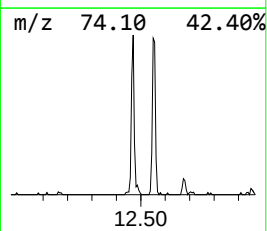
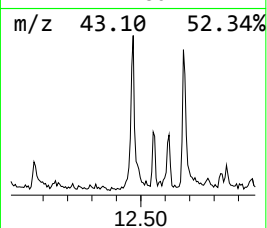
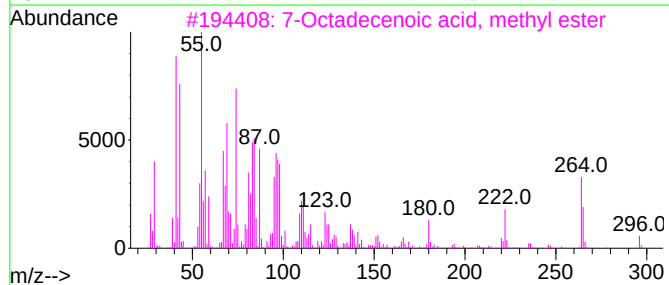
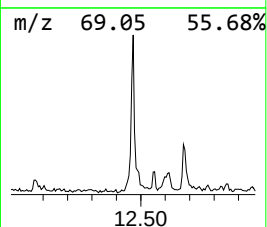
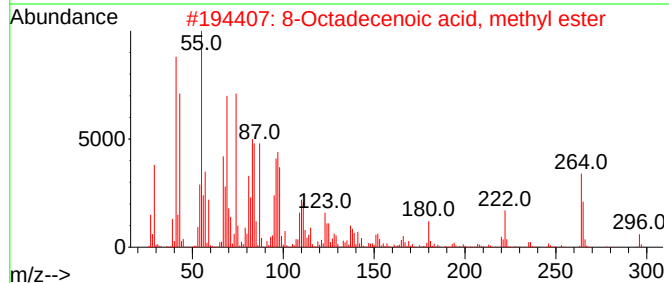
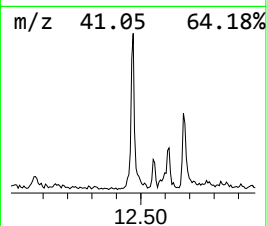
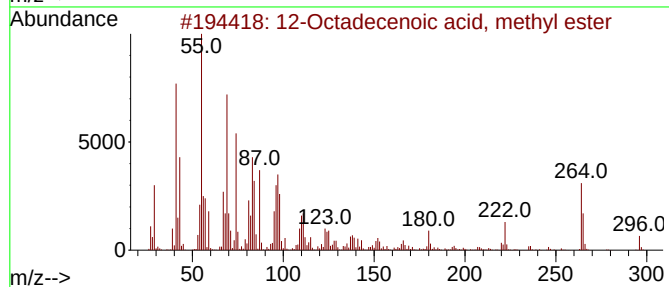
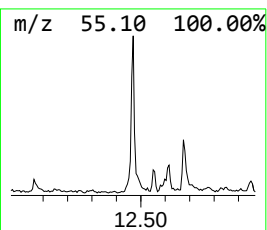
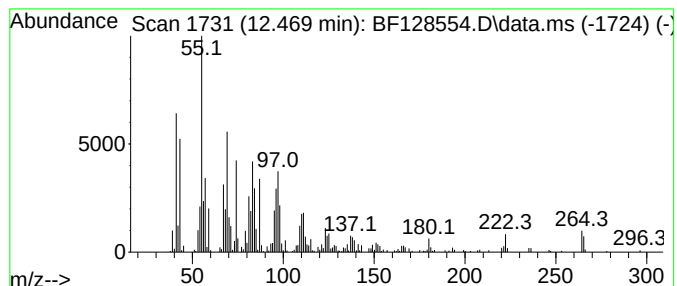
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 12-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	4.84 ng	361279	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2			8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	99
3			7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	97
4			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	97
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	97



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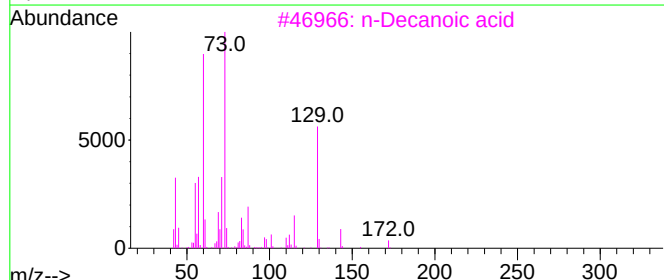
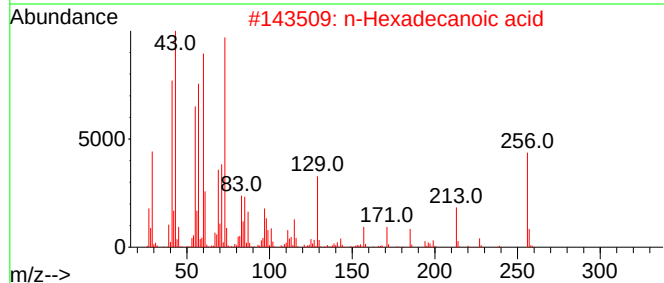
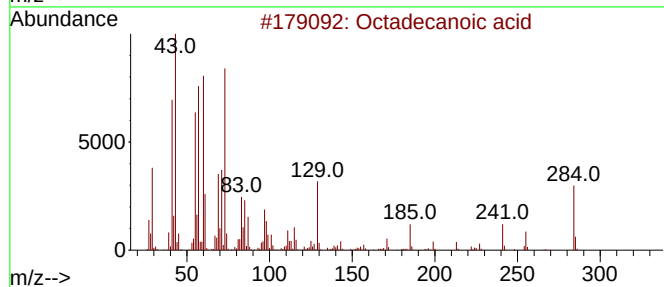
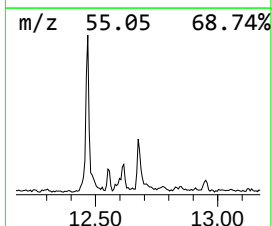
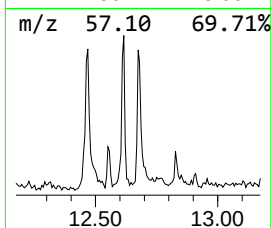
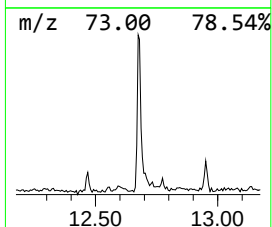
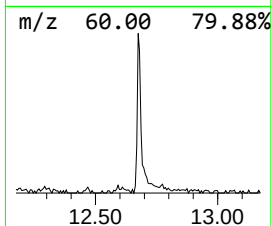
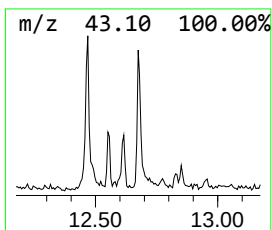
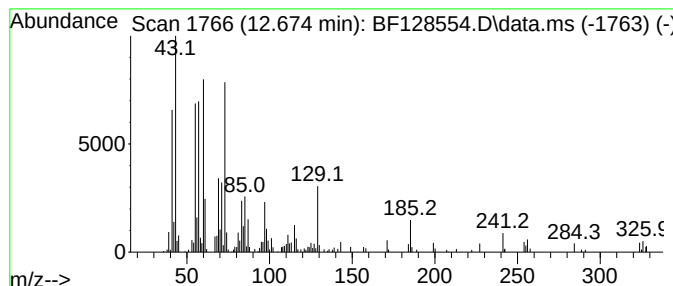
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.674	2.64 ng	196887	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	92
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Heneicosanoic acid, isopropyl ester	368	C24H48O2	1000405-13-6	80



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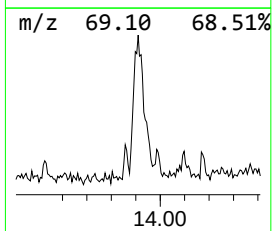
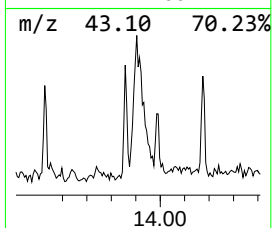
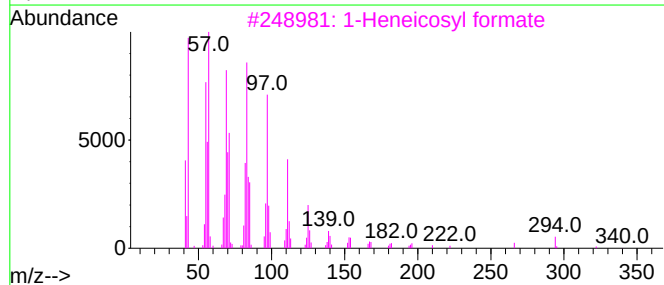
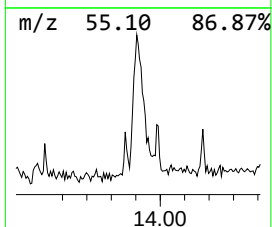
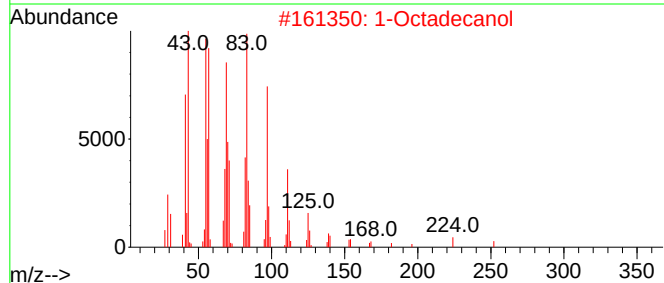
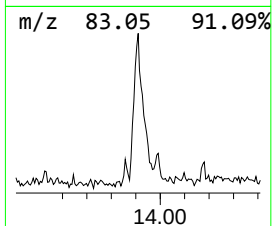
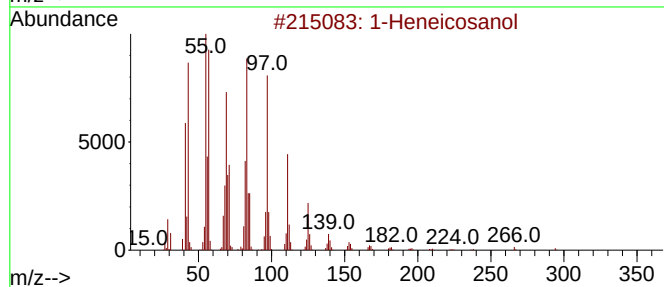
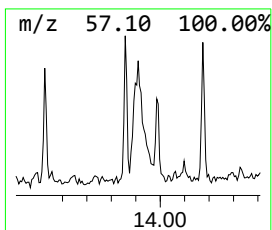
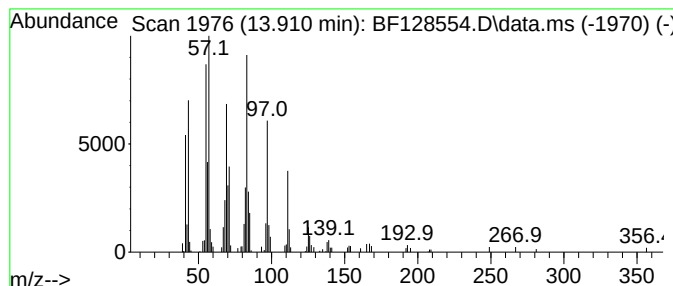
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Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	4.19 ng	221742	Chrysene-d12	13.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	91
2			1-Octadecanol	270	C18H38O	000112-92-5	90
3			1-Heneicosyl formate	340	C22H44O2	077899-03-7	83
4			1-Nonadecene	266	C19H38	018435-45-5	83
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	81



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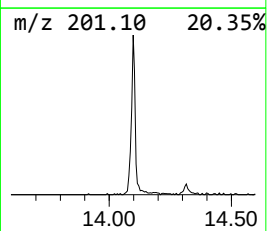
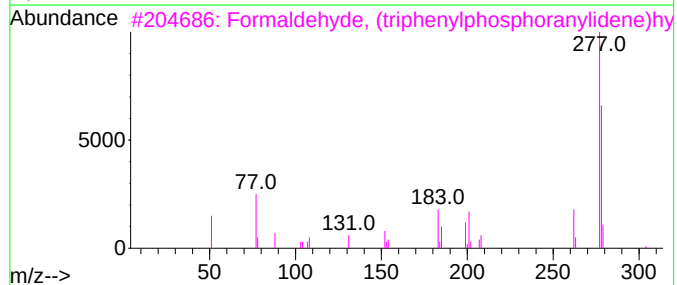
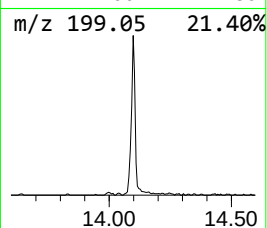
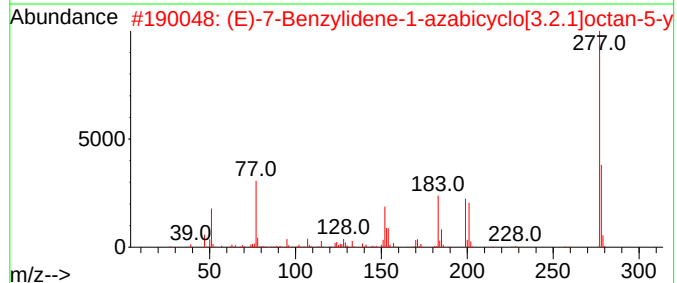
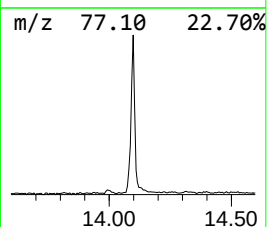
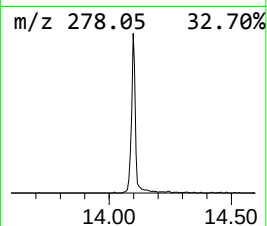
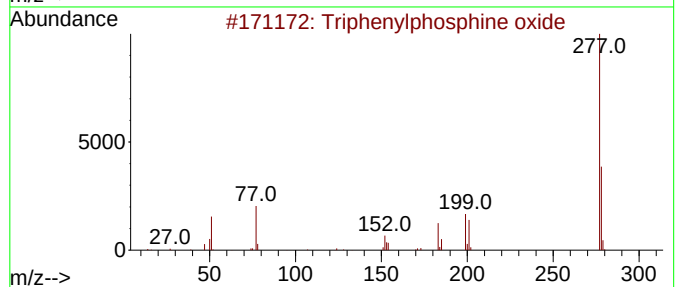
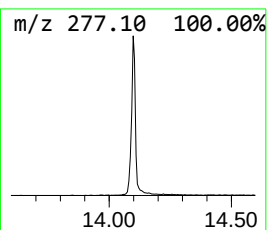
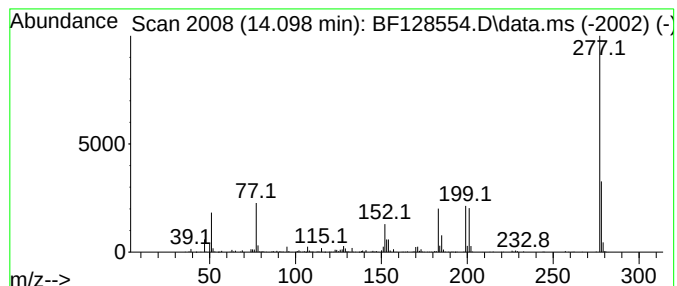
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.098	9.86 ng	522093	Chrysene-d12	13.998

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	45
4			Cobalt,(.eta.<5>-2,4-cyclopentad...	277	C16H15BCo	036682-12-9	32
5			Vanadium, cycloheptatrienyl-(pen...	277	C17H22V	1000155-20-5	9



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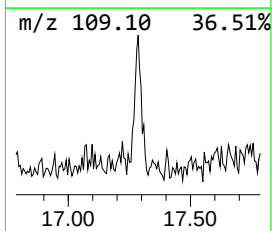
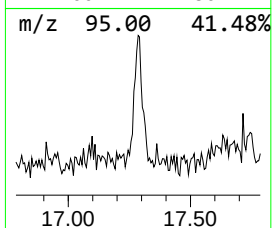
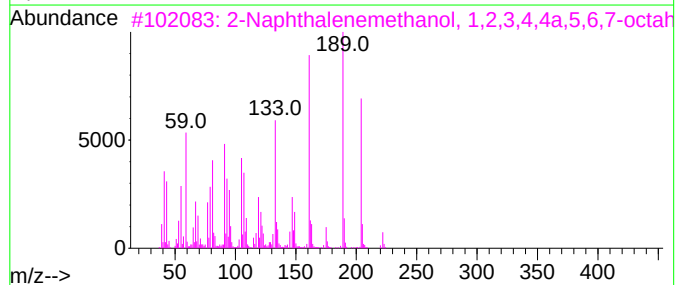
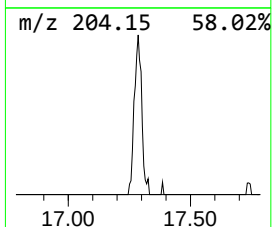
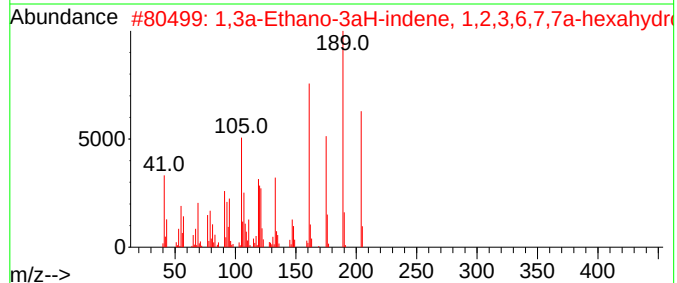
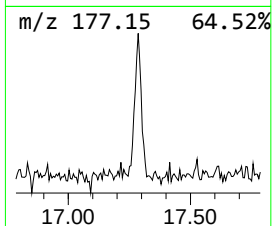
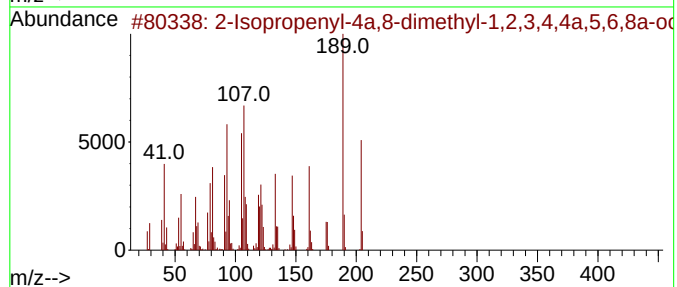
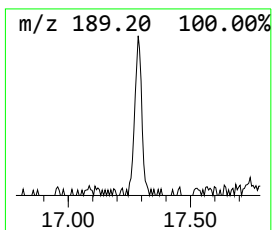
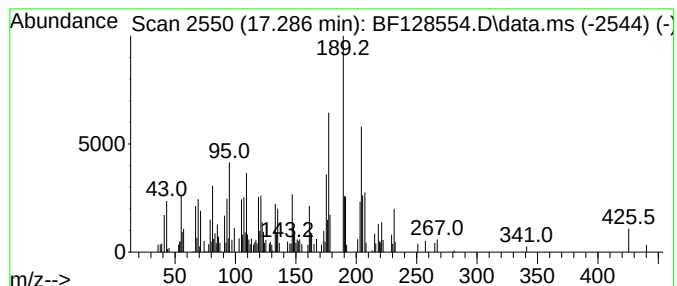
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Isopropenyl-4a,8-dimethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.286	2.85 ng	129552	Perylene-d12	15.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	84
2			1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	62
3			2-Naphthalenemethanol, 1,2,3,4,4...	222	C15H26O	001209-71-8	45
4			Cedrene-V6	204	C15H24	1000162-76-8	43
5			6-(4-Fluorophenyl)-2-hydroxypyri...	189	C11H8FNO	1010509-20-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF052822\
Data File : BF128554.D
Acq On : 28 May 2022 18:07
Operator : CG\JU
Sample : N2933-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
P023-SS003-0006-01

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.892	5.7	ng	425040	4	11.363	1491680	20.0
12-Octadecenoic...	12.469	4.8	ng	361279	4	11.363	1491680	20.0
Octadecanoic acid	12.674	2.6	ng	196887	4	11.363	1491680	20.0
1-Heneicosanol	13.910	4.2	ng	221742	5	13.998	1058770	20.0
Triphenylphosph...	14.098	9.9	ng	522093	5	13.998	1058770	20.0
2-Isopropenyl-4...	17.286	2.9	ng	129552	6	15.468	908144	20.0