

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125448.D
 Acq On : 13 Sep 2021 17:28
 Operator : JU/CG
 Sample : M3684-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DUP-210908A

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125448.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	11	18	27	rVV	1016285	1328053	36.77%	4.759%
2	2.305	31	37	42	rVB	46437	62002	1.72%	0.222%
3	5.110	509	514	521	rVB	130262	161391	4.47%	0.578%
4	5.510	578	582	600	rBV	2786784	2867378	79.39%	10.275%
5	6.522	749	754	770	rBV	2904170	2847635	78.84%	10.204%
6	6.881	812	815	819	rBV	957445	883539	24.46%	3.166%
7	7.445	906	911	922	rBV	1852651	1848726	51.19%	6.624%
8	8.075	1014	1018	1030	rBV	241569	521820	14.45%	1.870%
9	8.169	1030	1034	1037	rVV	1324827	1142863	31.64%	4.095%
10	9.245	1212	1217	1220	rBV	3650540	3228327	89.38%	11.568%
11	9.357	1232	1236	1241	rBV	65925	68766	1.90%	0.246%
12	9.928	1328	1333	1336	rBV	1534333	1303163	36.08%	4.670%
13	10.122	1362	1366	1375	rBV3	34543	56226	1.56%	0.201%
14	10.716	1463	1467	1471	rBV	2368115	2216890	61.38%	7.944%
15	11.416	1582	1586	1590	rBV	1723301	1407509	38.97%	5.043%
16	11.798	1646	1651	1654	rBV	48969	43414	1.20%	0.156%
17	11.939	1668	1675	1691	rBV	907978	1098539	30.42%	3.936%
18	12.504	1766	1771	1775	rBV	101172	102166	2.83%	0.366%
19	12.722	1803	1808	1818	rBV	470893	531162	14.71%	1.903%
20	13.004	1852	1856	1859	rBV	4171803	3611739	100.00%	12.942%
21	13.957	2010	2018	2030	rBV7	53951	167078	4.63%	0.599%
22	14.063	2032	2036	2040	rBV	1320196	1187672	32.88%	4.256%
23	14.374	2084	2089	2096	rVB10	16486	39817	1.10%	0.143%
24	14.833	2162	2167	2170	rBV	46851	72427	2.01%	0.260%
25	15.174	2222	2225	2229	rVB	42853	46648	1.29%	0.167%
26	15.557	2285	2290	2298	rBV2	716909	964715	26.71%	3.457%
27	16.015	2363	2368	2372	rVB3	35806	53877	1.49%	0.193%
28	16.527	2451	2455	2461	rVB4	24840	44081	1.22%	0.158%

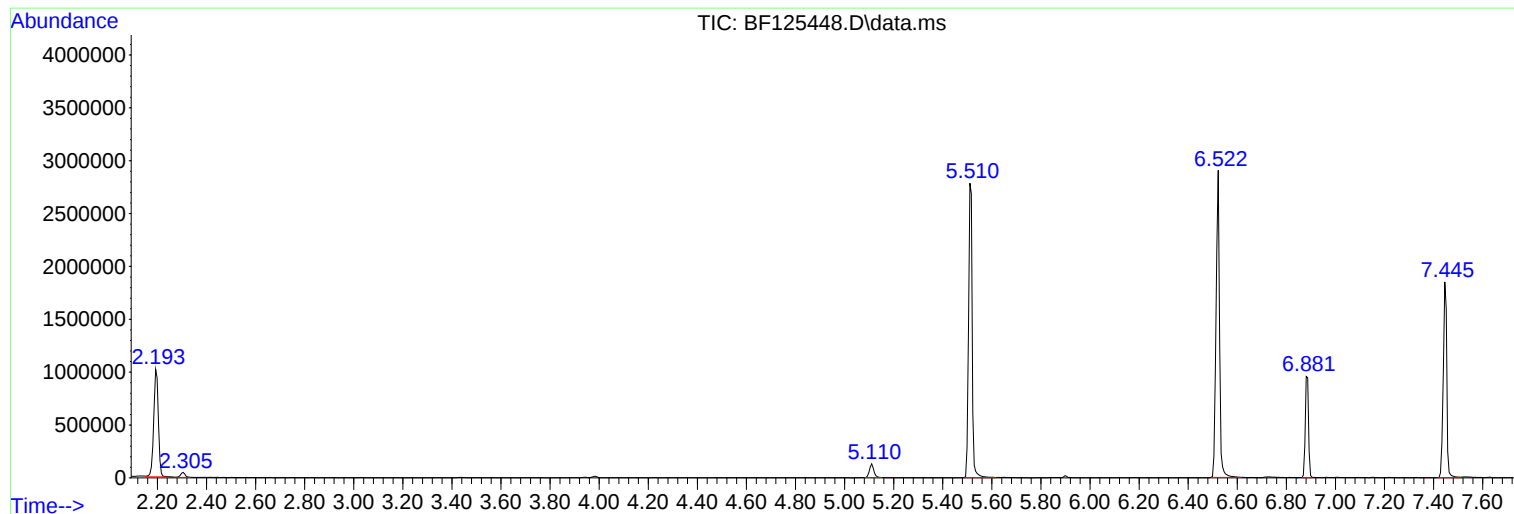
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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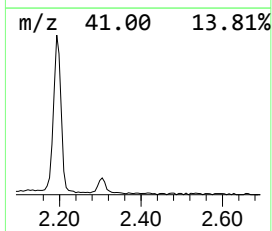
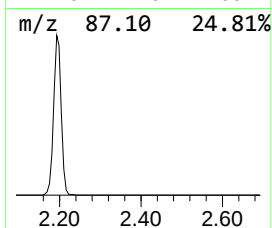
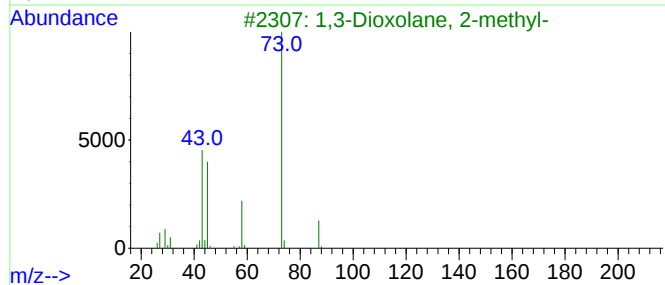
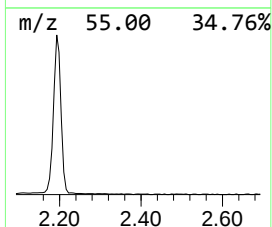
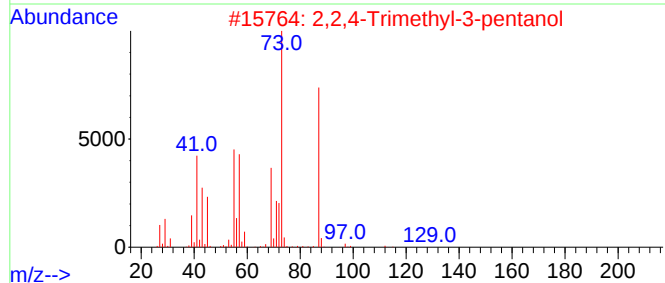
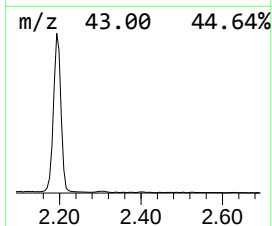
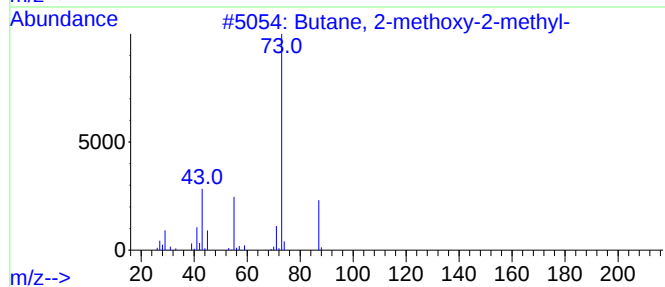
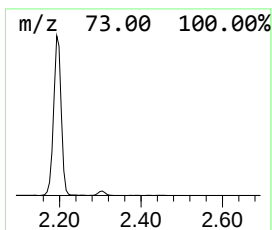
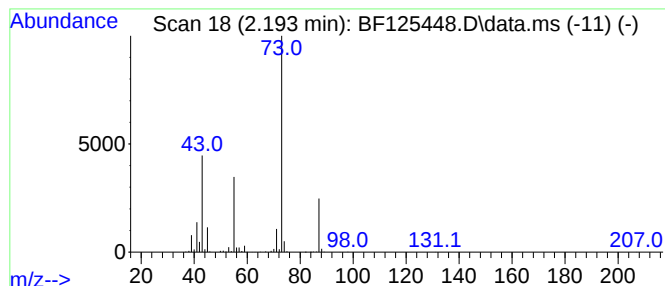
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.193	30.06 ng	1328050	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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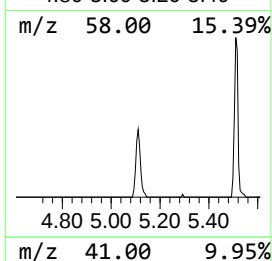
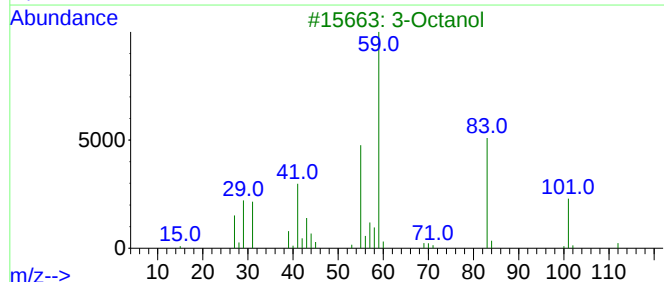
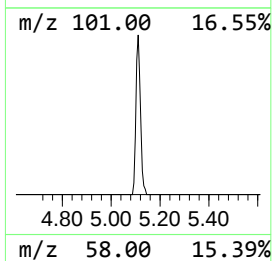
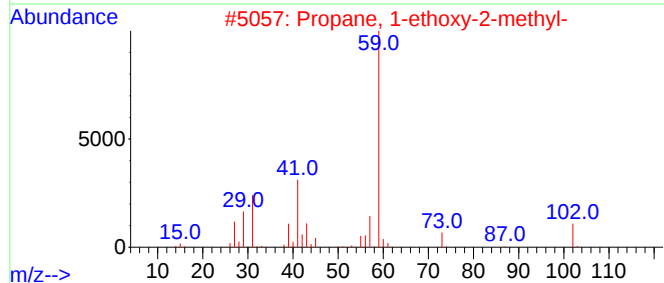
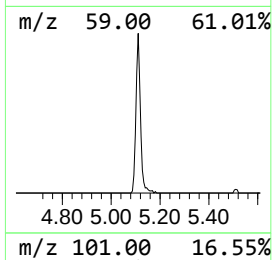
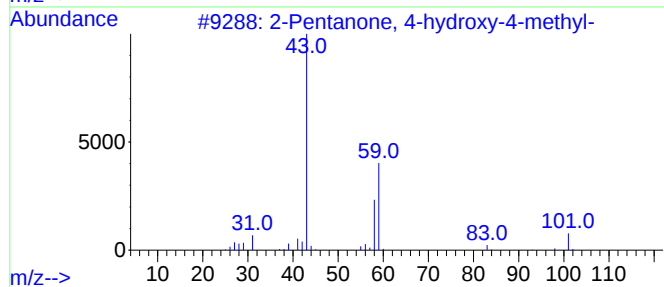
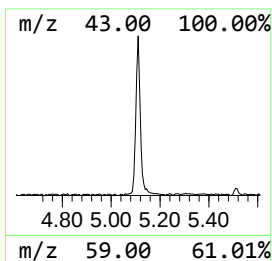
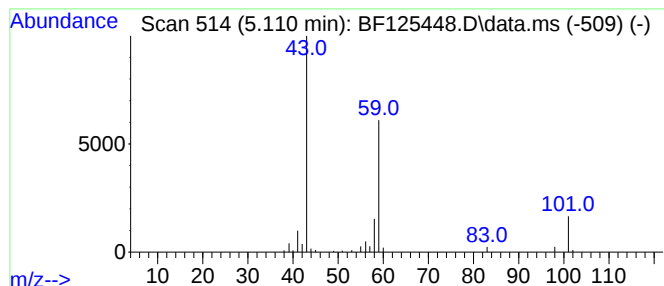
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.65 ng	161391	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	46
3			3-Octanol	130	C8H18O	000589-98-0	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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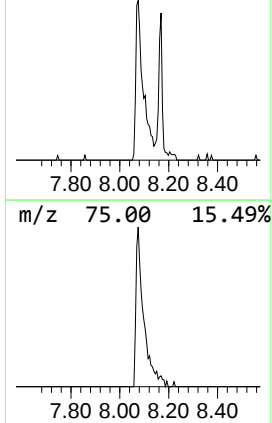
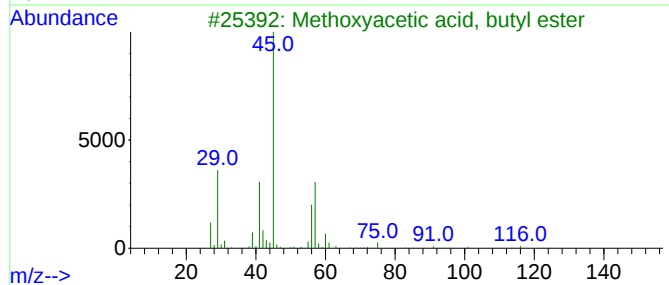
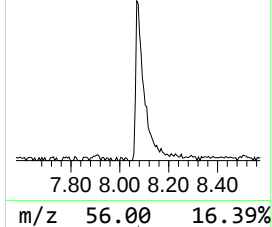
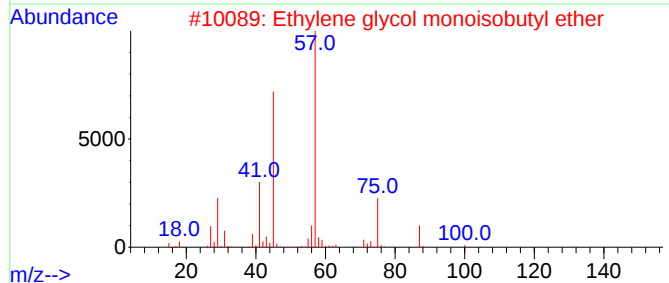
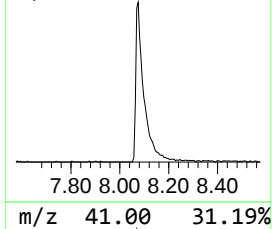
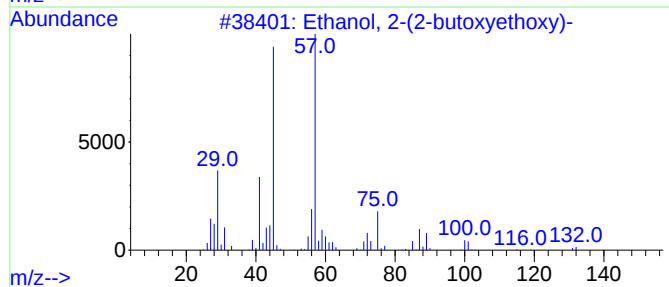
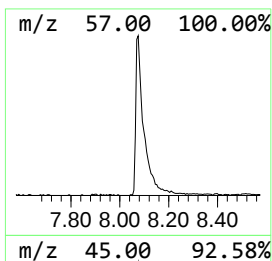
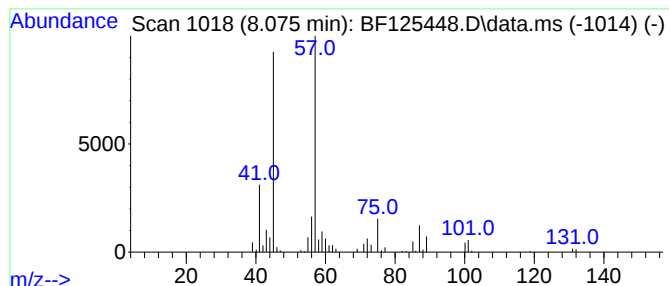
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	9.13 ng	521820	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3			Methoxyacetic acid, butyl ester	146	C7H14O3	017640-22-1	53
4			Tetraethylene glycol	194	C8H18O5	000112-60-7	53
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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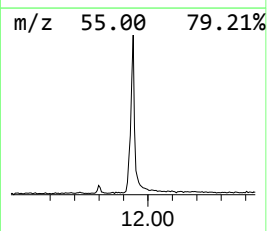
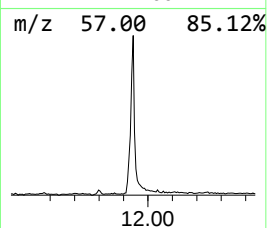
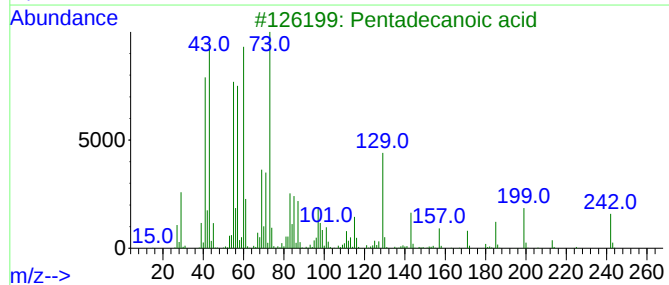
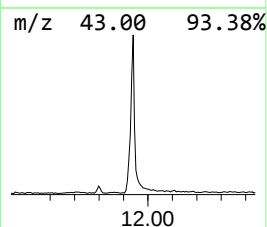
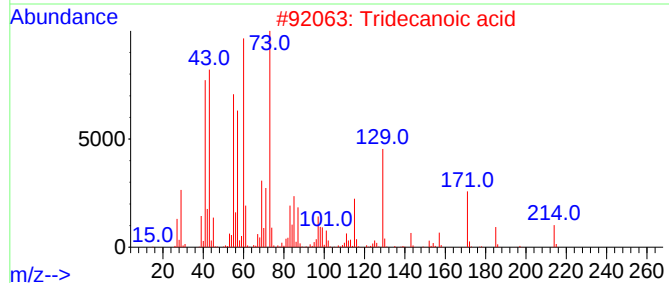
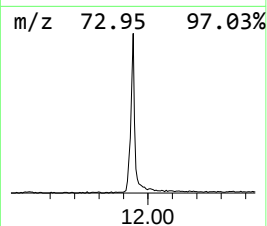
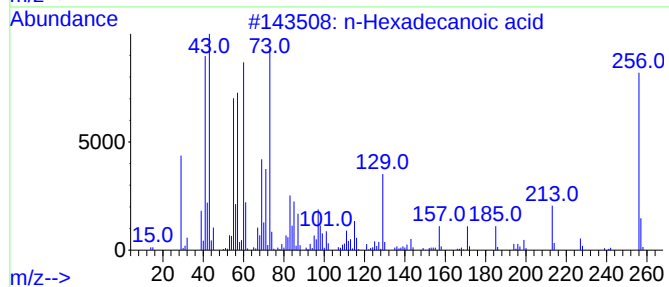
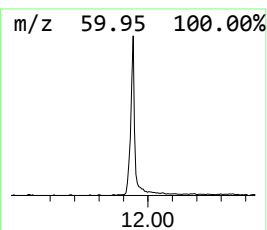
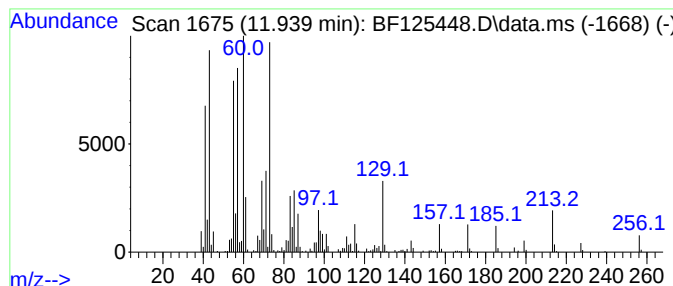
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	15.61 ng	1098540	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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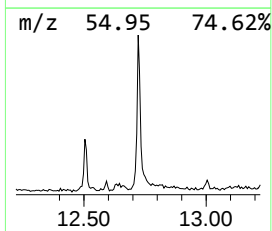
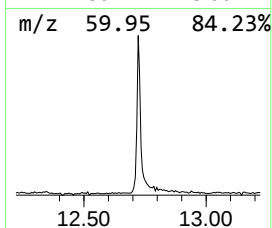
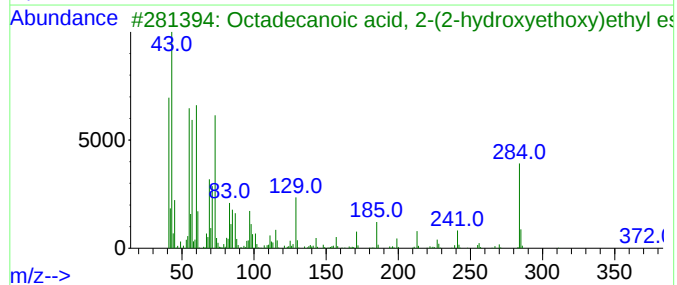
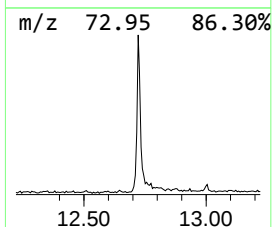
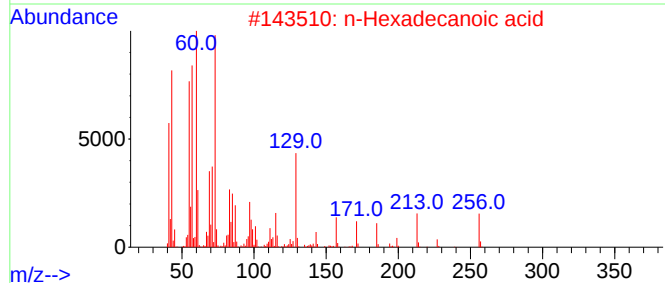
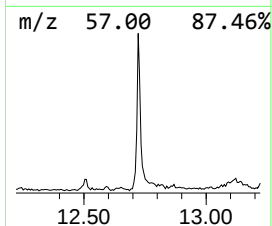
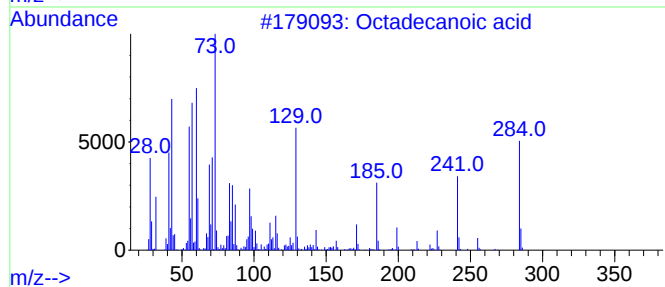
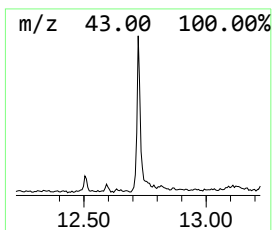
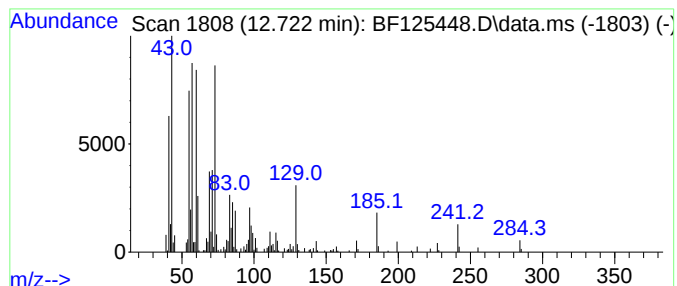
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.722	7.55 ng	531162	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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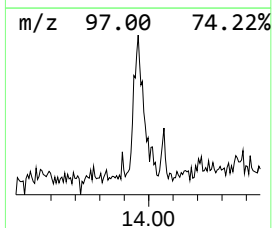
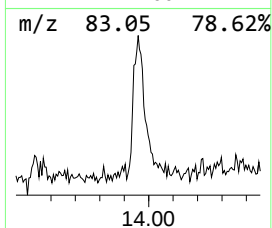
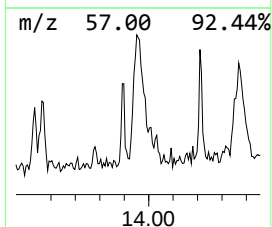
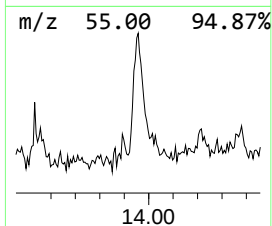
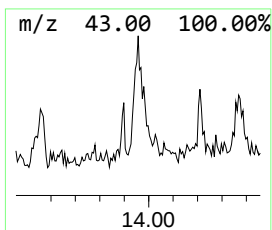
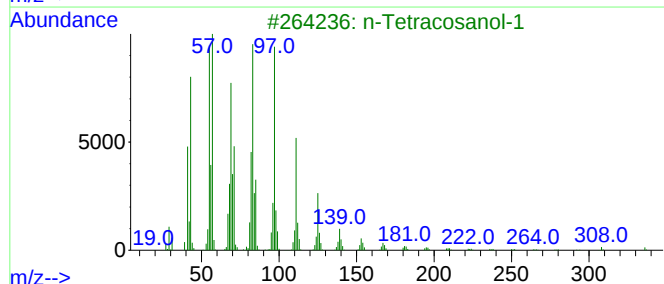
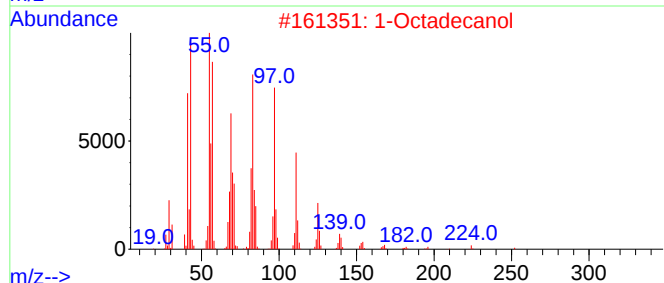
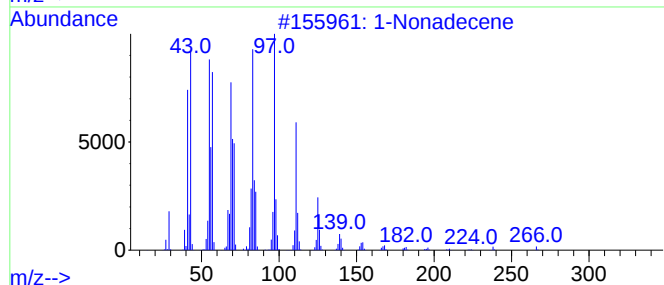
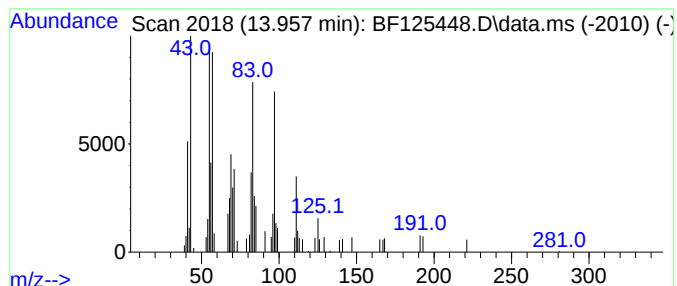
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Nonadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	2.81 ng	167078	Chrysene-d12	14.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	90
2	1-Octadecanol		270	C18H38O	000112-92-5	90
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	87
4	Behenic alcohol		326	C22H46O	000661-19-8	87
5	1-Docosene		308	C22H44	001599-67-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
Data File : BF125448.D
Acq On : 13 Sep 2021 17:28
Operator : JU/CG
Sample : M3684-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-210908A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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
Butane, 2-metho...	2.193	30.1	ng	1328050	1	6.887	883539	20.0
2-Pentanone, 4-...	5.110	3.6	ng	161391	1	6.887	883539	20.0
Ethanol, 2-(2-b...	8.075	9.1	ng	521820	2	8.169	1142860	20.0
n-Hexadecanoic ...	11.939	15.6	ng	1098540	4	11.416	1407510	20.0
Octadecanoic acid	12.722	7.5	ng	531162	4	11.416	1407510	20.0
1-Nonadecene	13.957	2.8	ng	167078	5	14.063	1187670	20.0