

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
 Data File : BF123364.D
 Acq On : 3 Mar 2021 19:47
 Operator : JU/CG
 Sample : M1545-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 4

Instrument :
 BNA_F
 ClientSampleId :
 MH-J

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-BF021921.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123364.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.869	128	133	136	rVB	4865306	6181026	40.43%	5.817%
2	3.352	211	215	221	rVB	343578	491704	3.22%	0.463%
3	5.575	588	593	596	rBV	6127862	6413362	41.95%	6.035%
4	5.740	618	621	628	rVB	348316	305966	2.00%	0.288%
5	6.516	747	753	769	rBV2	2864341	4770666	31.20%	4.490%
6	6.857	806	811	818	rBV	2812130	2829704	18.51%	2.663%
7	7.269	875	881	888	rVB	106706	170687	1.12%	0.161%
8	7.422	898	907	910	rBV	5046169	9478237	61.99%	8.920%
9	8.128	1019	1027	1031	rBV	2273658	3865430	25.28%	3.638%
10	8.851	1144	1150	1156	rBV	299813	349677	2.29%	0.329%
11	8.957	1162	1168	1177	rBV3	85554	191005	1.25%	0.180%
12	9.210	1201	1211	1214	rBV	7163522	15289834	100.00%	14.389%
13	9.604	1270	1278	1282	rBV2	167311	289851	1.90%	0.273%
14	9.816	1306	1314	1317	rBV3	140742	306594	2.01%	0.289%
15	9.886	1317	1326	1330	rVB	2677505	4477822	29.29%	4.214%
16	10.692	1451	1463	1466	rBV	5568217	10068997	65.85%	9.476%
17	11.386	1570	1581	1583	rBV	3341506	4422652	28.93%	4.162%
18	11.933	1661	1674	1682	rBV	3188502	4654312	30.44%	4.380%
19	12.198	1716	1719	1724	rVB	194778	233952	1.53%	0.220%
20	12.357	1743	1746	1749	rVV	860247	741592	4.85%	0.698%
21	12.410	1753	1755	1760	rVB	171580	174731	1.14%	0.164%
22	12.610	1785	1789	1791	rBV2	264828	324856	2.12%	0.306%
23	12.716	1802	1807	1813	rBV	2420950	2458731	16.08%	2.314%
24	12.992	1841	1854	1857	rBV2	8736074	14523042	94.98%	13.667%
25	13.186	1884	1887	1892	rBV3	127523	190033	1.24%	0.179%
26	13.874	2000	2004	2015	rVB	2889414	3080547	20.15%	2.899%
27	14.045	2027	2033	2035	rBV	3716798	3912663	25.59%	3.682%
28	14.192	2056	2058	2066	rVB2	189313	225586	1.48%	0.212%
29	14.498	2107	2110	2111	rBV	216806	204391	1.34%	0.192%
30	14.804	2160	2162	2165	rVB	197801	175804	1.15%	0.165%
31	15.145	2217	2220	2223	rVB	236964	237662	1.55%	0.224%
32	15.527	2277	2285	2289	rBV	2829029	4076166	26.66%	3.836%
33	15.963	2355	2359	2364	rBV2	166295	246222	1.61%	0.232%
34	16.027	2365	2370	2379	rBV	418258	897589	5.87%	0.845%

Sum of corrected areas: 106261093

Instrument :

BNA_F

ClientSampleId :

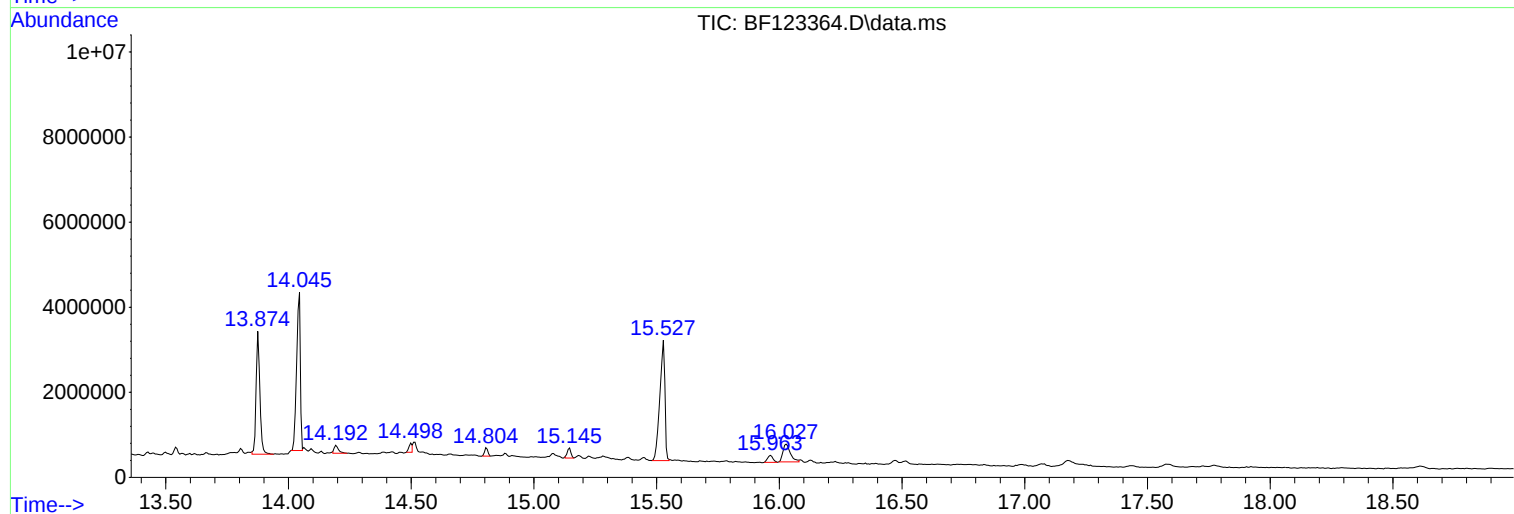
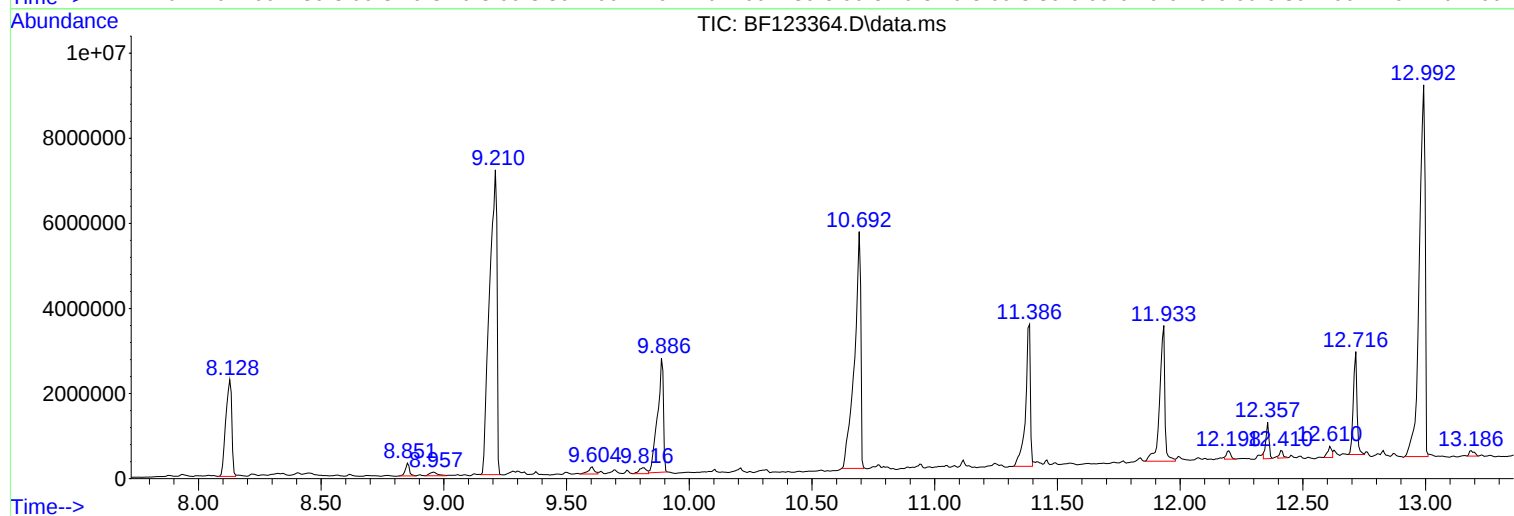
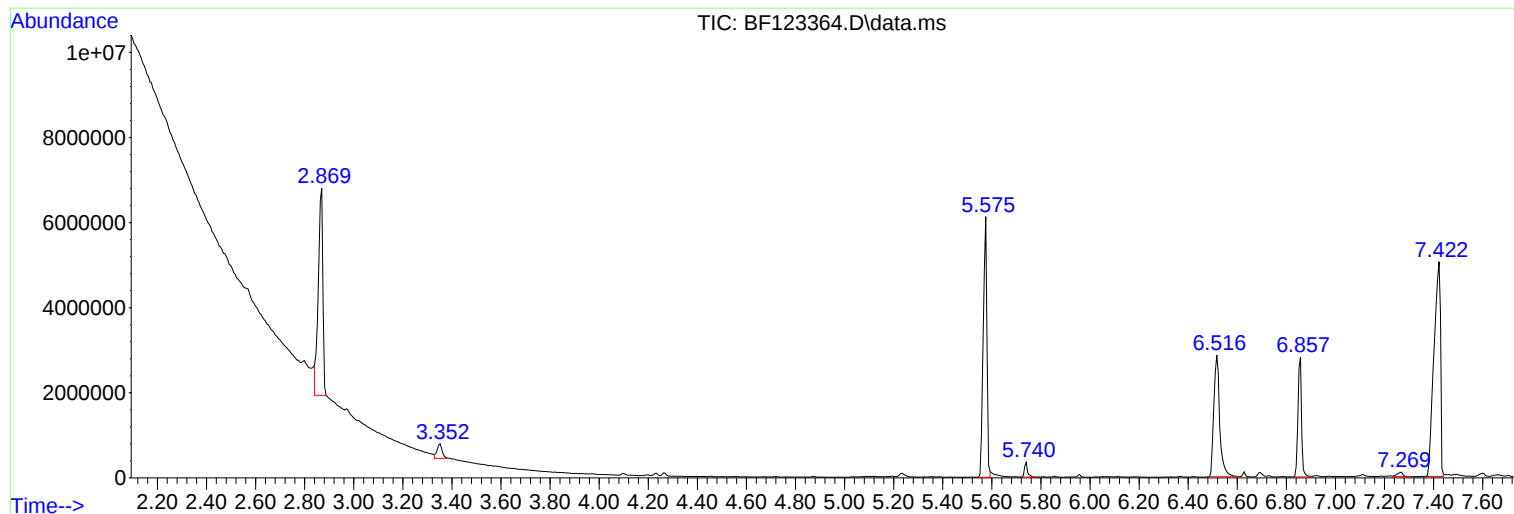
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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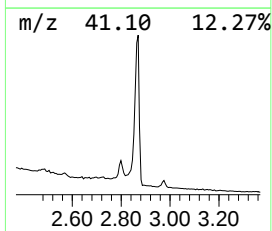
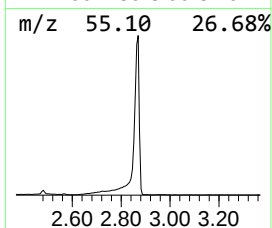
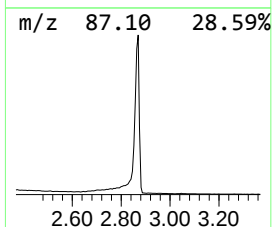
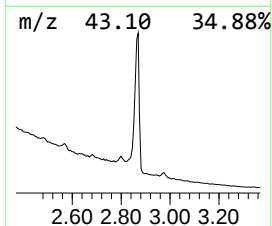
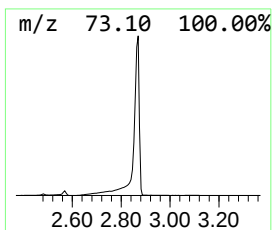
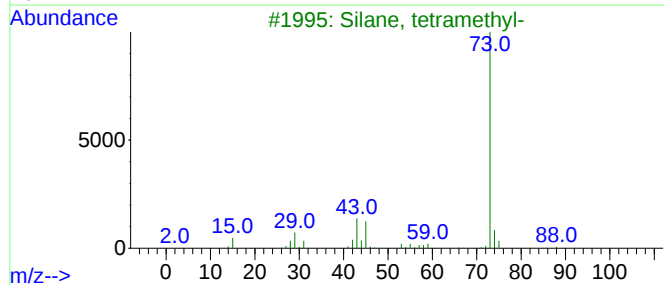
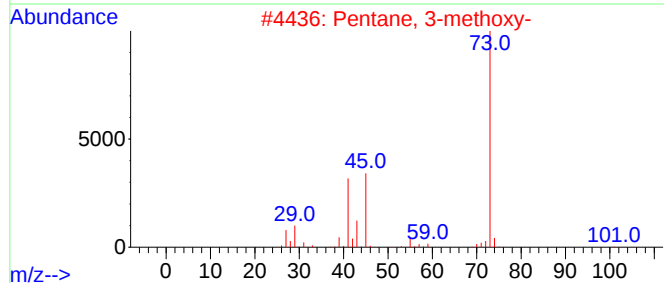
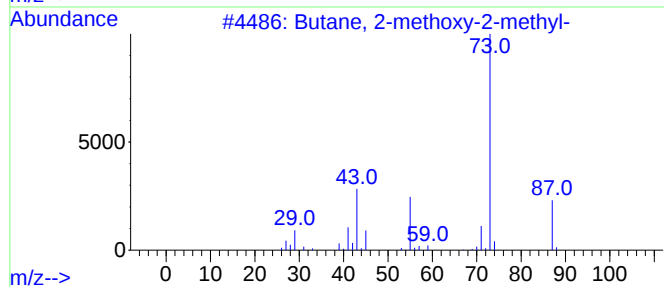
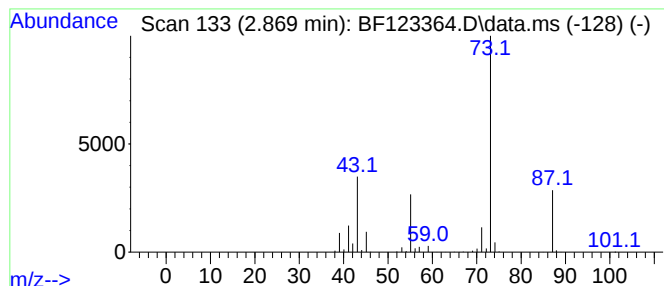
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.869	43.69 ng	6181030	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
4			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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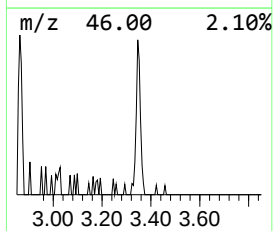
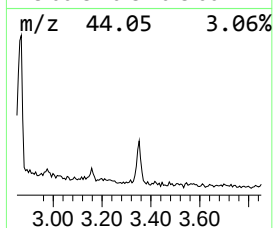
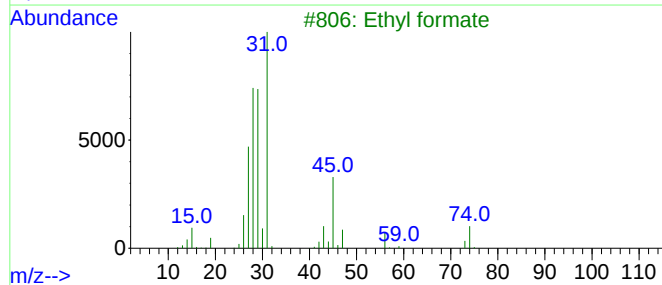
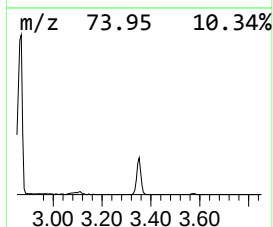
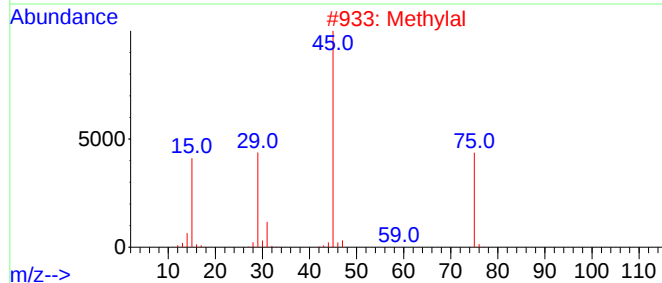
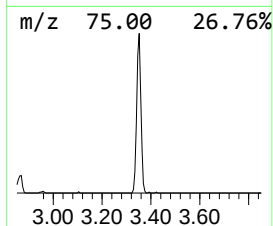
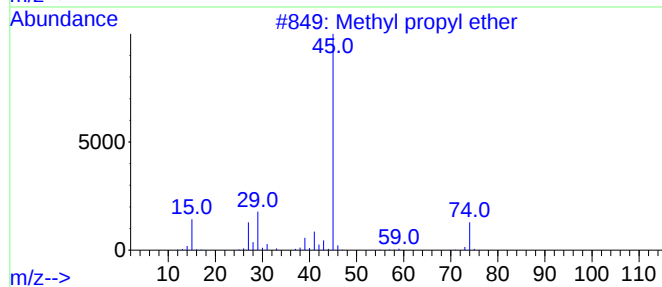
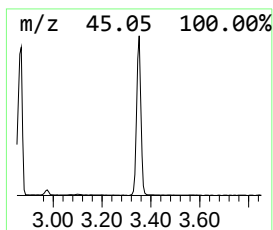
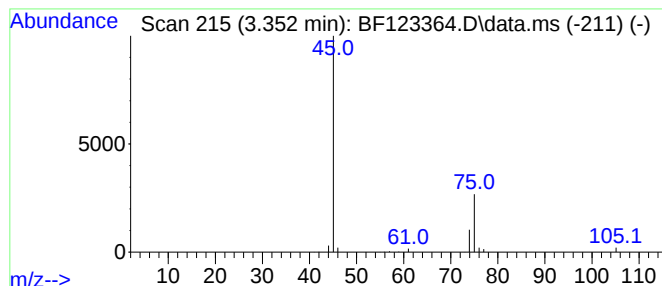
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.352 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.352	3.48 ng	491704	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl propyl ether	74	C4H10O	000557-17-5	7
2			Methylal	76	C3H8O2	000109-87-5	7
3			Ethyl formate	74	C3H6O2	000109-94-4	4
4			Formamide	45	CH3NO	000075-12-7	4
5			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	4



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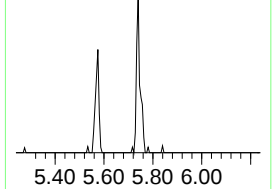
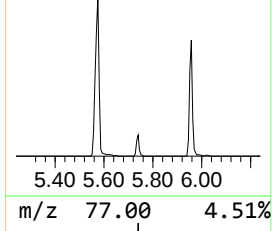
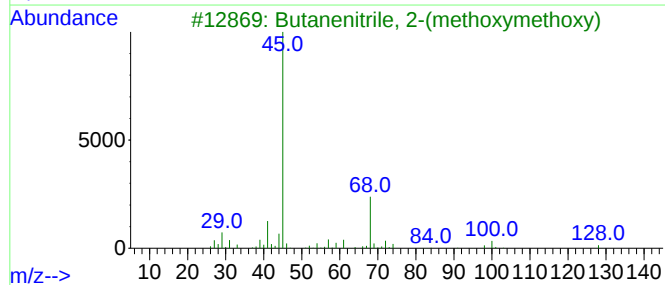
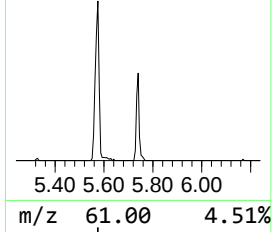
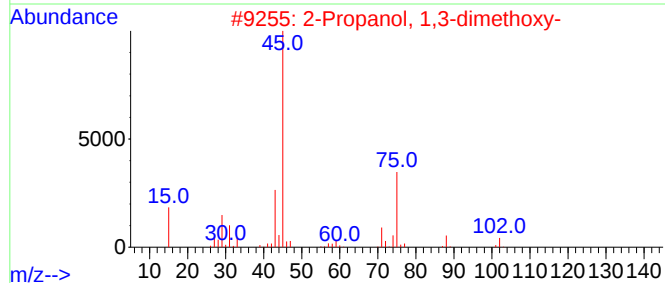
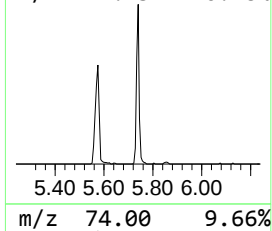
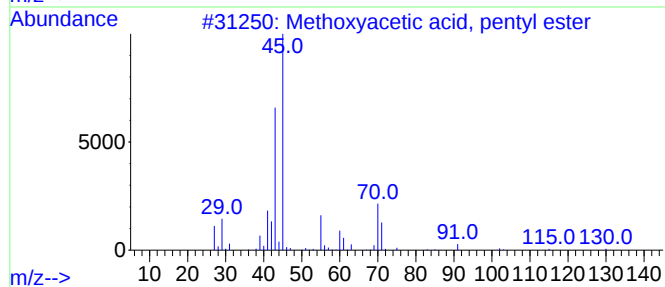
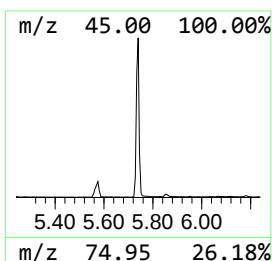
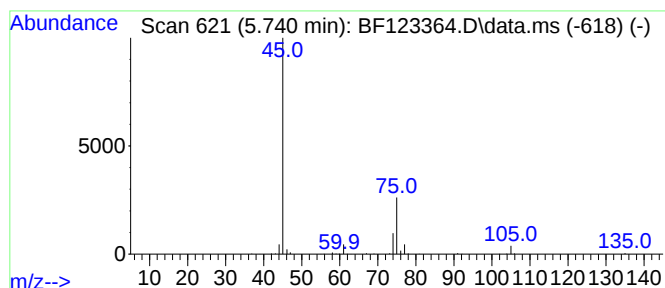
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown5.740 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.740	2.16 ng	305966	1,4-Dichlorobenzene-d4	6.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	9
2			2-Propanol, 1,3-dimethoxy-	120	C5H12O3	000623-69-8	9
3			Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
4			Hexane, 1-(methoxymethoxy)-	146	C8H18O2	066675-06-7	9
5			Methyl propyl ether	74	C4H10O	000557-17-5	7



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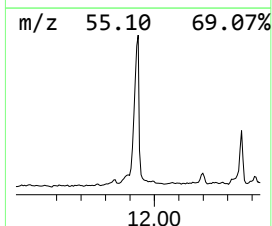
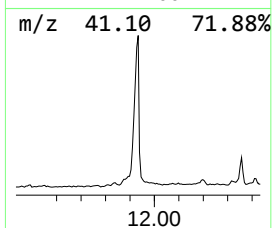
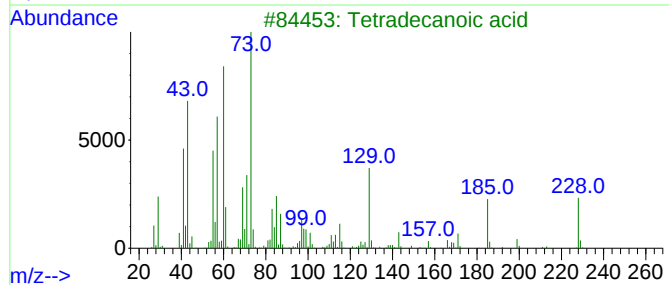
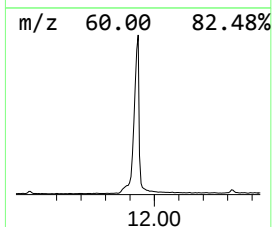
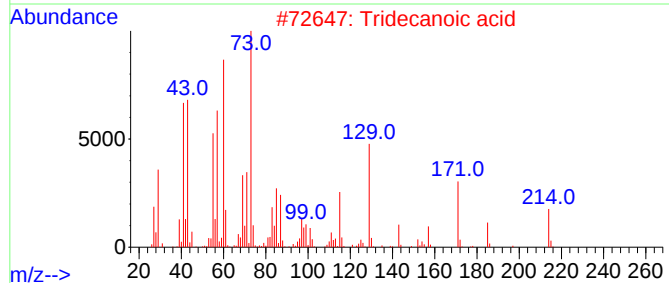
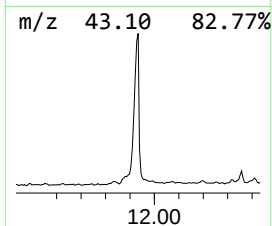
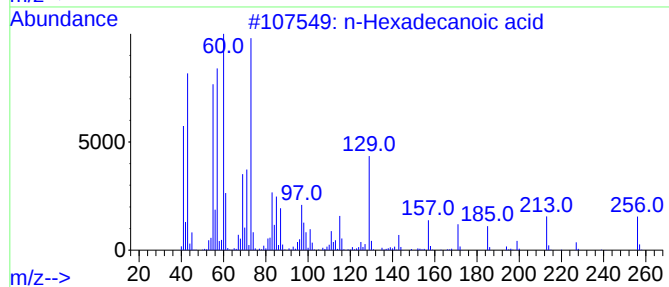
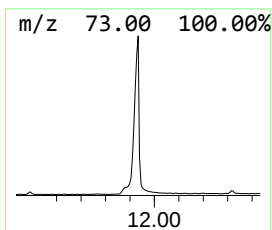
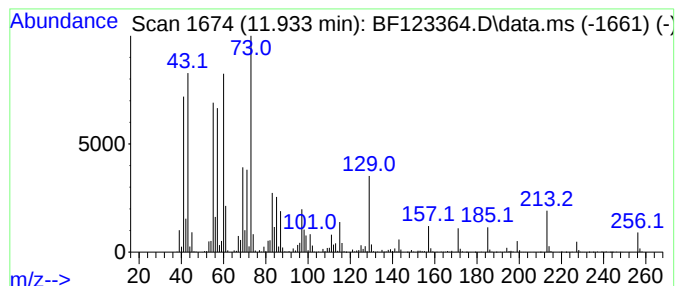
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.933	21.05 ng	4654310	Phenanthrene-d10		11.386	
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	92
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
5	Estra-1,3,5(10)-trien-17.β.-ol		256	C18H24O	002529-64-8	30



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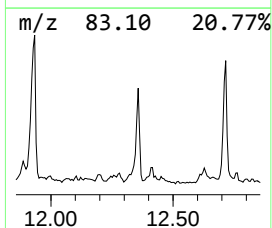
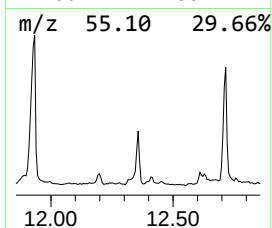
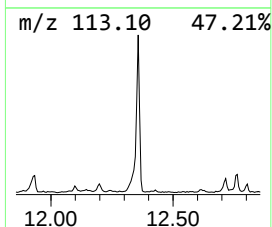
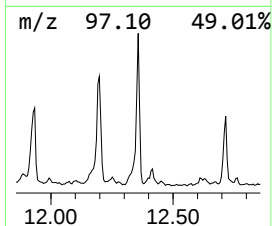
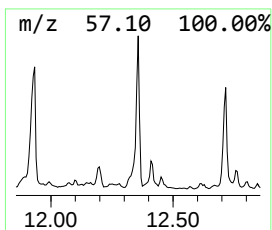
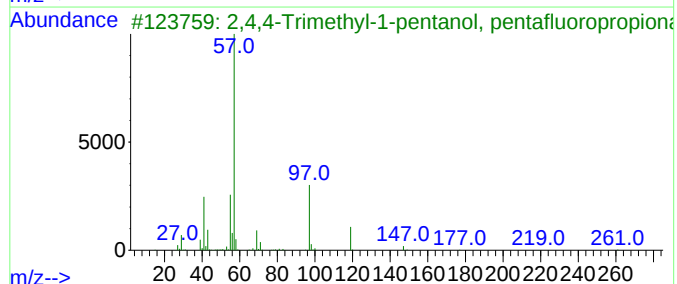
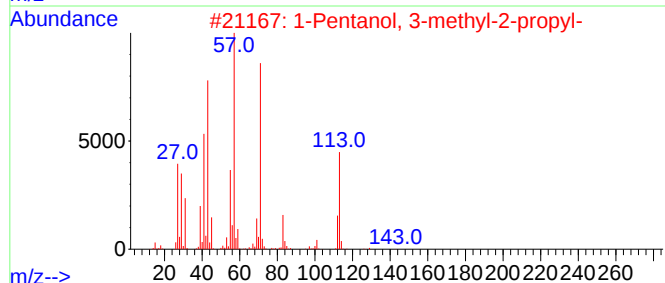
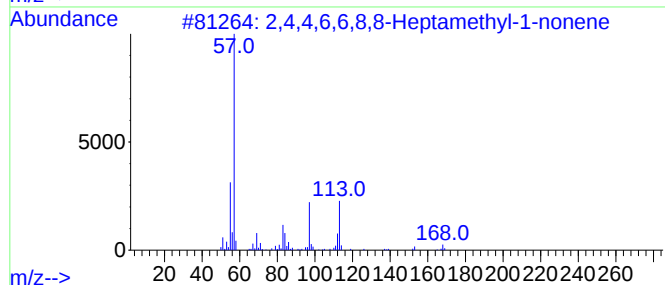
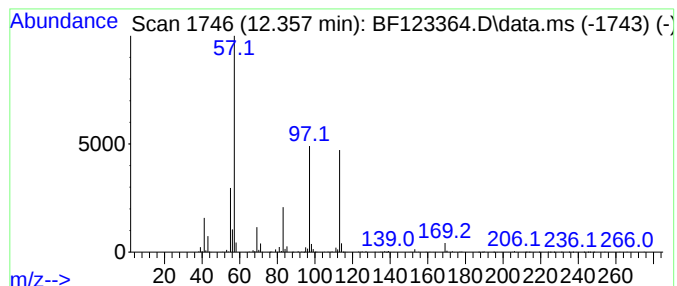
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown12.357 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	3.35 ng	741592	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38		
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	33		
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	27		
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25		
5	4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	25		



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Sample : M1545-07
Misc :
ALS Vial : 13 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-J

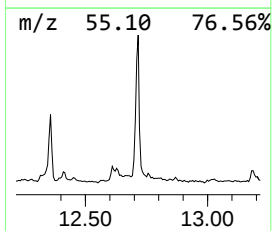
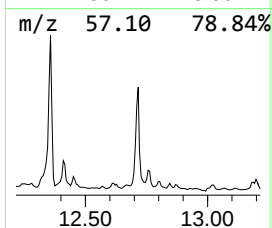
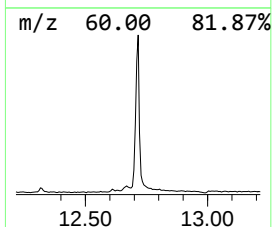
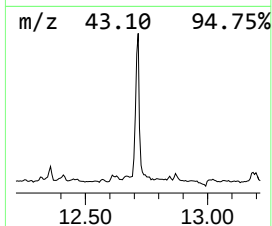
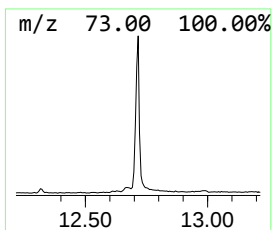
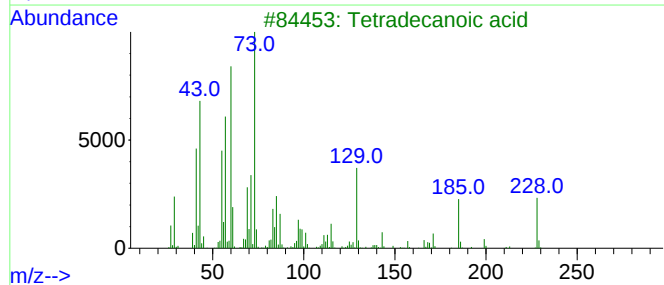
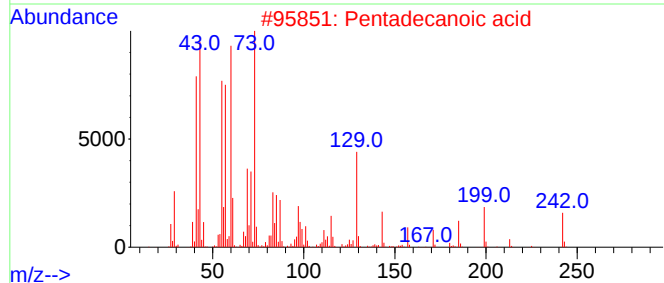
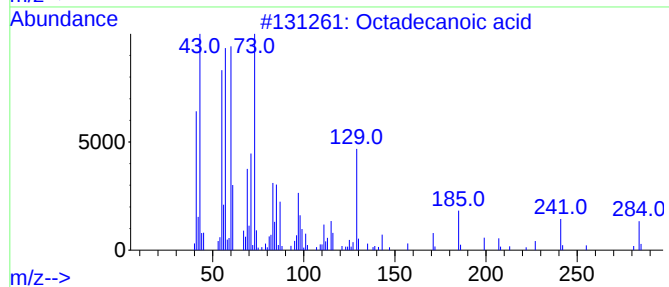
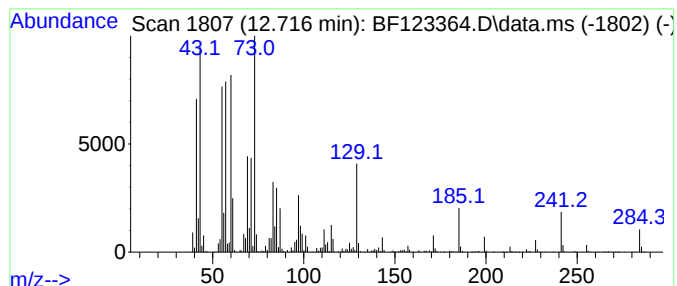
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	12.57 ng	2458730	Chrysene-d12	14.045

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123364.D
Acq On : 3 Mar 2021 19:47
Operator : JU/CG
Sample : M1545-07
Misc :
ALS Vial : 13 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-J

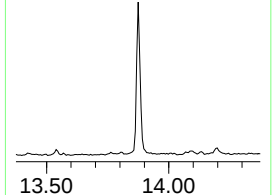
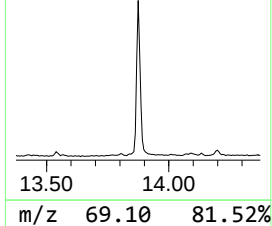
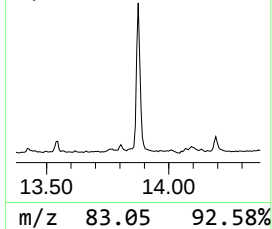
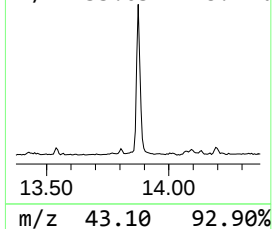
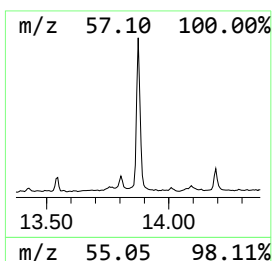
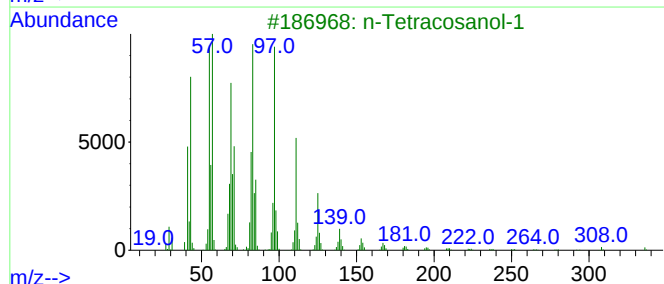
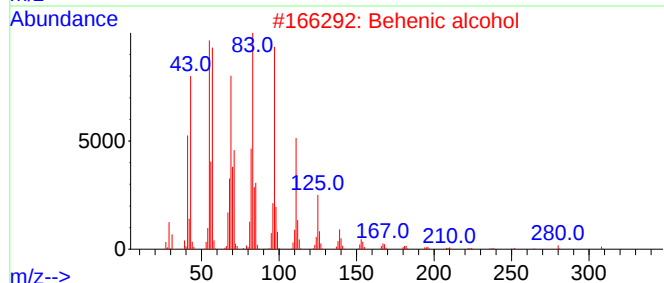
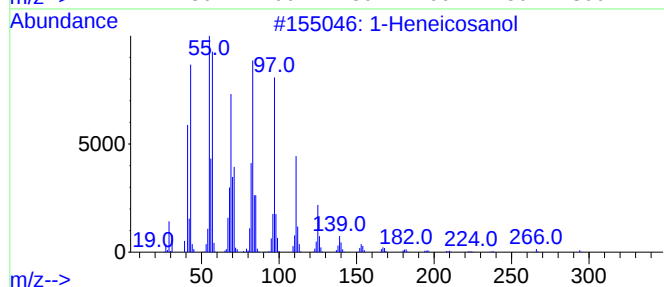
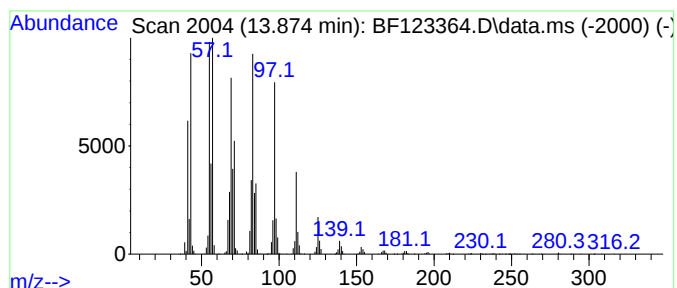
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	15.75 ng	3080550	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			1-Nonadecene	266	C19H38	018435-45-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
Data File : BF123364.D
Acq On : 3 Mar 2021 19:47
Operator : JU/CG
Sample : M1545-07
Misc :
ALS Vial : 13 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-J

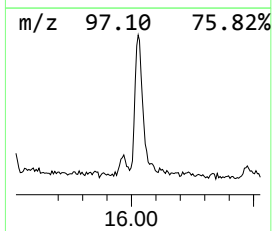
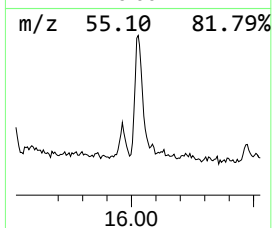
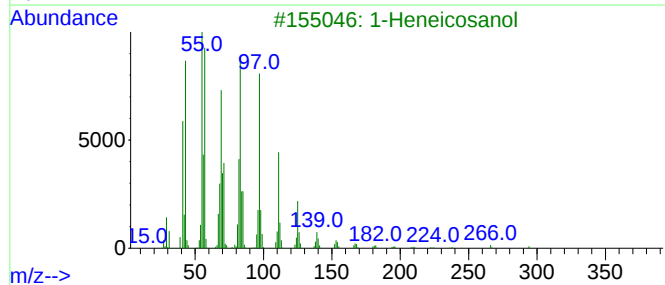
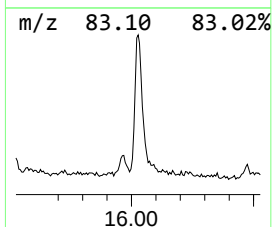
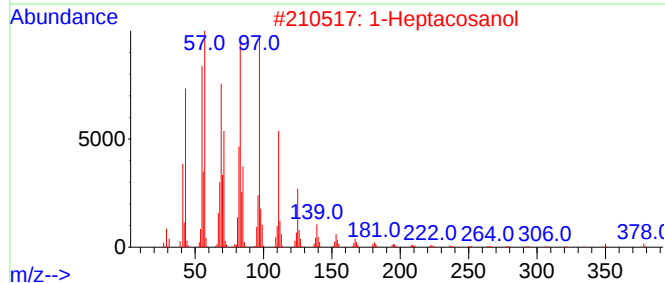
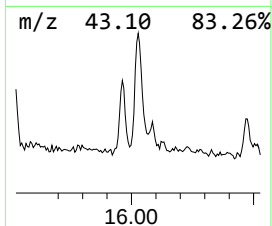
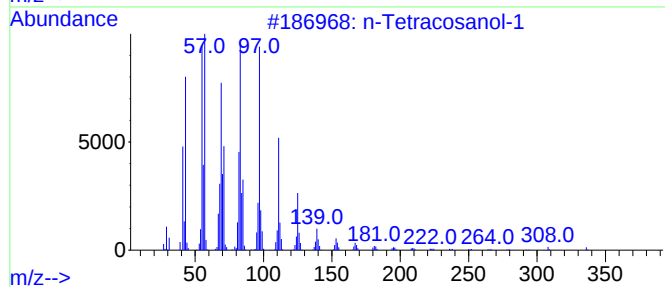
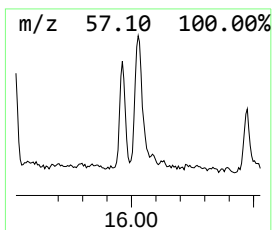
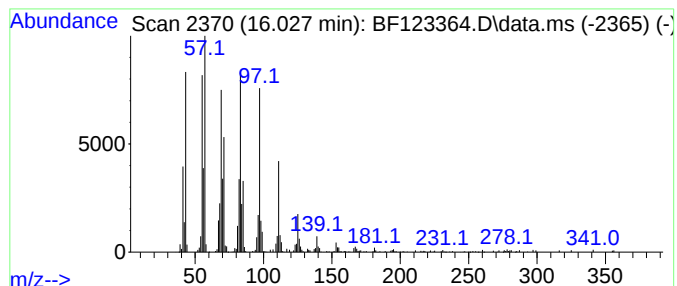
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.027	4.40 ng	897589	Perylene-d12	15.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2			1-Heptacosanol	396	C27H56O	002004-39-9	91
3			1-Heneicosanol	312	C21H44O	015594-90-8	90
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
5			Octacosanol	410	C28H58O	000557-61-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030321\
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Acq On : 3 Mar 2021 19:47
Operator : JU/CG
Sample : M1545-07
Misc :
ALS Vial : 13 Sample Multiplier: 4

Instrument :
BNA_F
ClientSampleId :
MH-J

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF021921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.869	43.7	ng	6181030	1	6.857	2829700	20.0
unknown3.352	3.352	3.5	ng	491704	1	6.857	2829700	20.0
unknown5.740	5.740	2.2	ng	305966	1	6.857	2829700	20.0
n-Hexadecanoic ...	11.933	21.1	ng	4654310	4	11.386	4422650	20.0
unknown12.357	12.357	3.4	ng	741592	4	11.386	4422650	20.0
Octadecanoic acid	12.716	12.6	ng	2458730	5	14.045	3912660	20.0
1-Heneicosanol	13.874	15.8	ng	3080550	5	14.045	3912660	20.0
n-Tetracosanol-1	16.027	4.4	ng	897589	6	15.527	4076170	20.0