

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
 Data File : BF123979.D
 Acq On : 18 May 2021 15:25
 Operator : JU/CG
 Sample : M2435-10
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HOMESTEAD-B

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-BF051421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123979.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	11	19	25	rVB	661291	825981	51.42%	7.142%
2	5.522	579	584	587	rBV	1455085	1298233	80.82%	11.225%
3	6.387	727	731	735	rBV4	16002	31678	1.97%	0.274%
4	6.528	749	755	758	rBV	1290476	1344089	83.67%	11.622%
5	6.728	786	789	794	rBV	27934	28262	1.76%	0.244%
6	6.904	815	819	822	rBV	439523	324561	20.20%	2.806%
7	7.463	909	914	917	rBV	917883	901188	56.10%	7.792%
8	8.186	1033	1037	1040	rBV	518636	412435	25.68%	3.566%
9	9.263	1215	1220	1223	rBV	1924858	1606362	100.00%	13.889%
10	9.651	1283	1286	1290	rBV	192910	169379	10.54%	1.465%
11	9.945	1332	1336	1339	rBV	631946	489677	30.48%	4.234%
12	10.733	1465	1470	1473	rBV	1197881	1084779	67.53%	9.380%
13	11.174	1541	1545	1549	rBV2	16773	19281	1.20%	0.167%
14	11.427	1585	1588	1592	rBV	537903	487652	30.36%	4.216%
15	11.951	1674	1677	1681	rBV2	98612	91844	5.72%	0.794%
16	12.739	1808	1811	1815	rBV4	22439	27467	1.71%	0.237%
17	13.021	1854	1859	1862	rBV	1372429	1325731	82.53%	11.463%
18	13.915	2008	2011	2019	rBV	138071	198127	12.33%	1.713%
19	14.068	2034	2037	2041	rVB	326896	311394	19.39%	2.692%
20	14.233	2063	2065	2071	rVB6	15887	20814	1.30%	0.180%
21	14.545	2112	2118	2119	rBV5	35733	43696	2.72%	0.378%
22	14.857	2168	2171	2176	rVB3	36678	41730	2.60%	0.361%
23	14.998	2190	2195	2198	rBV6	15217	34171	2.13%	0.295%
24	15.209	2227	2231	2236	rBV4	39381	58439	3.64%	0.505%
25	15.568	2286	2292	2296	rBV	233495	325913	20.29%	2.818%
26	16.051	2370	2374	2379	rBV5	23159	41719	2.60%	0.361%
27	16.115	2382	2385	2387	rBV4	16677	20820	1.30%	0.180%

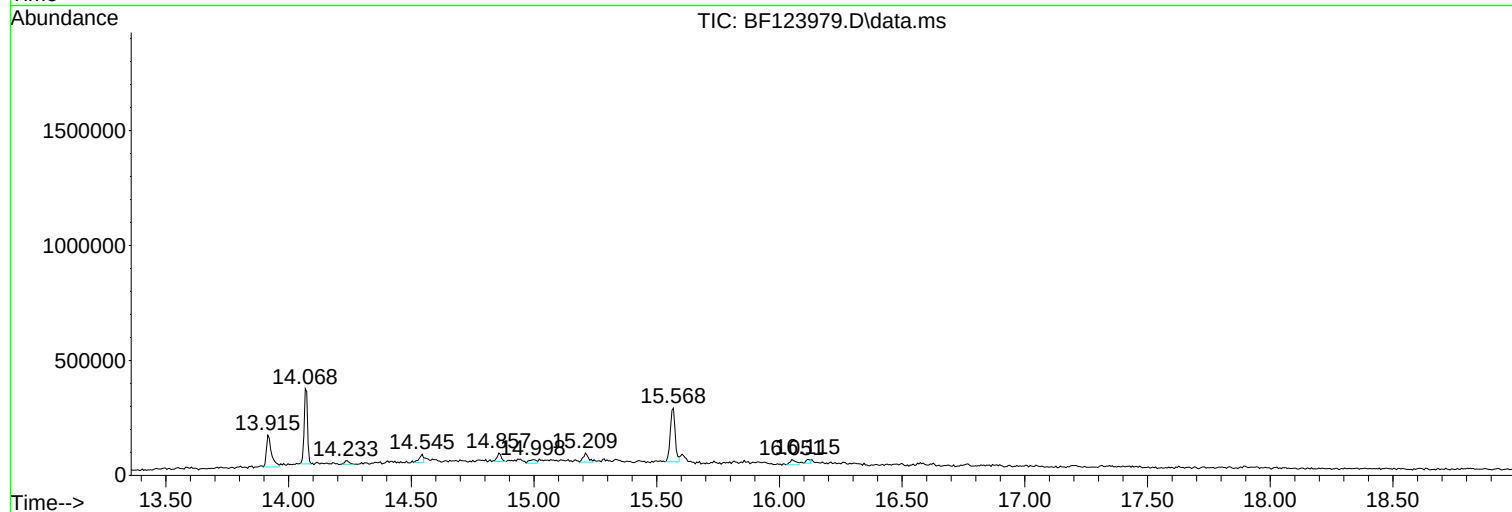
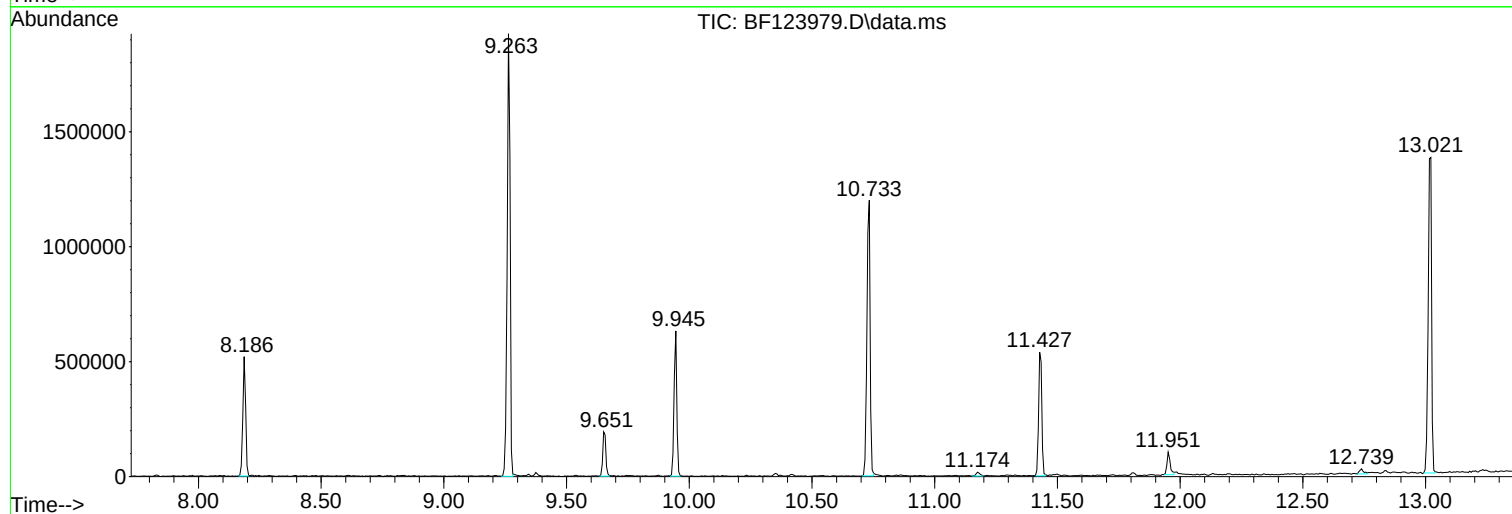
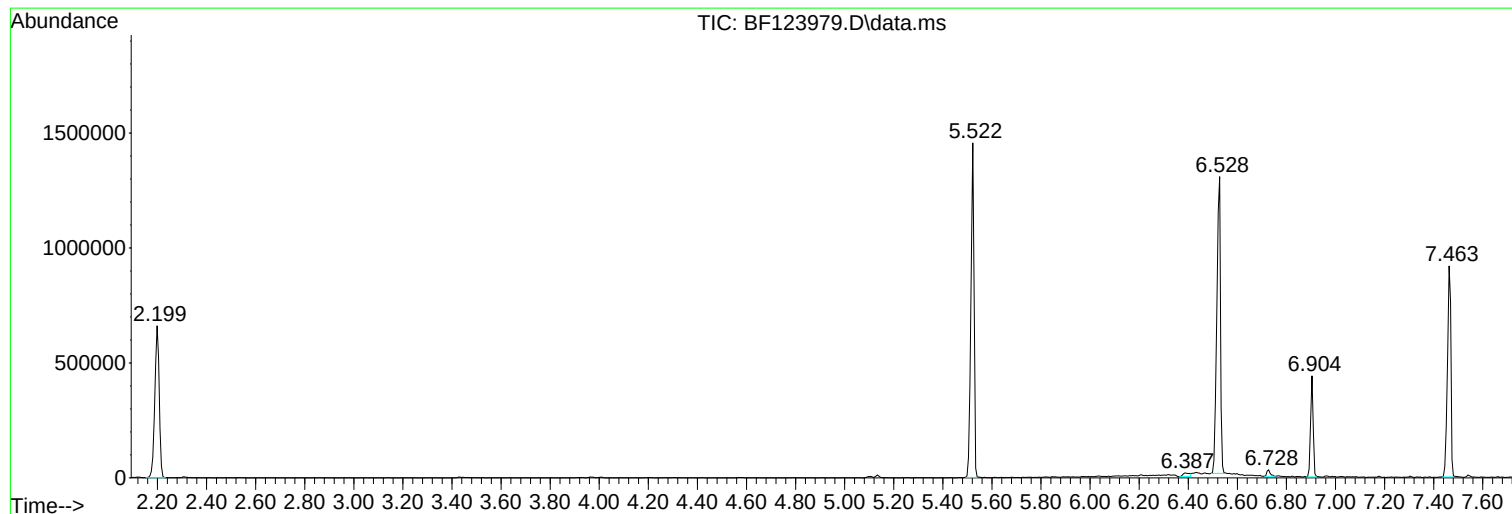
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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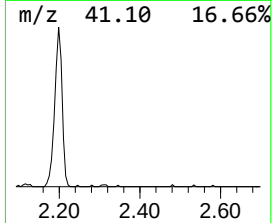
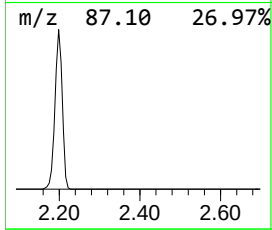
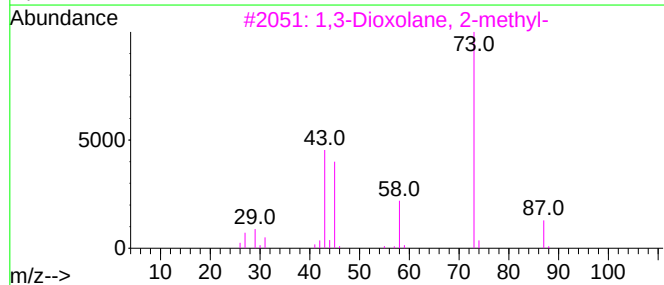
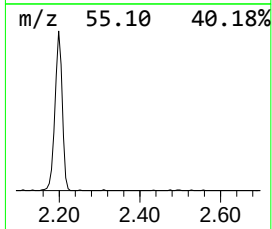
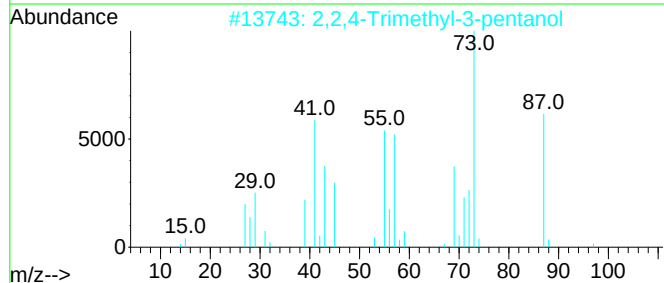
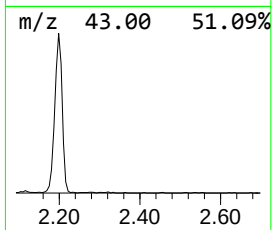
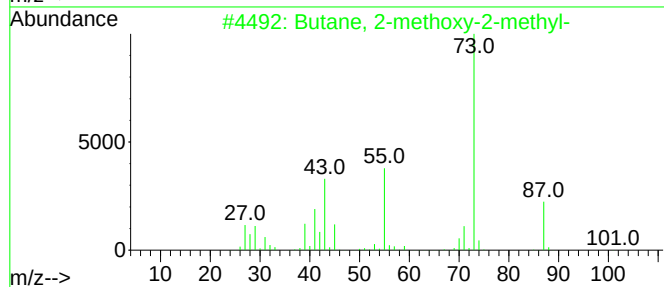
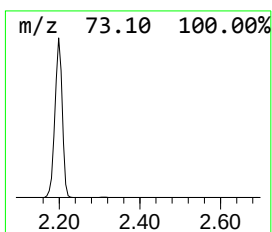
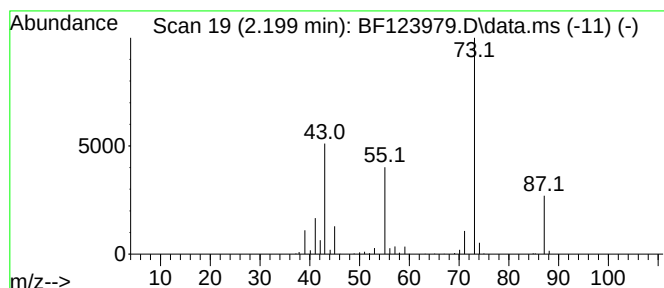
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	50.90 ng	825981	1,4-Dichlorobenzene-d4	6.904

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	9
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9



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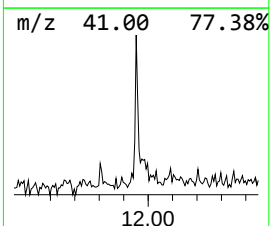
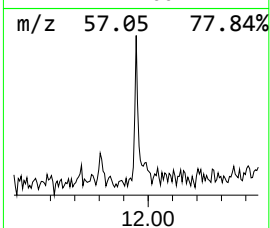
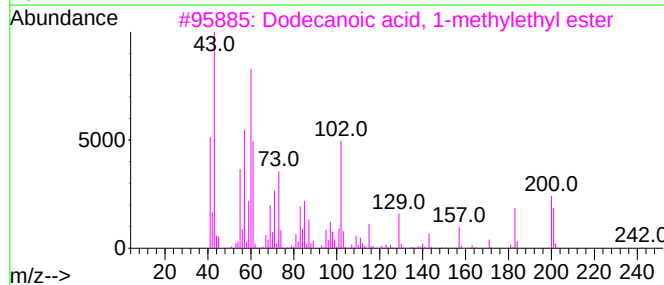
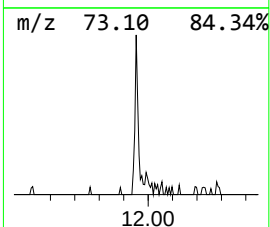
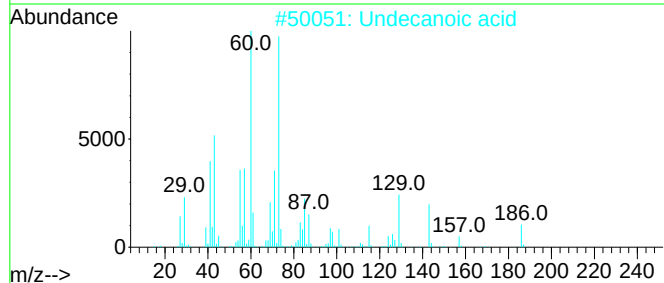
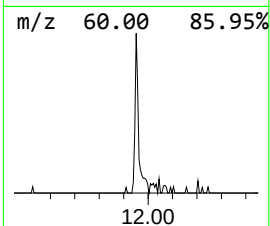
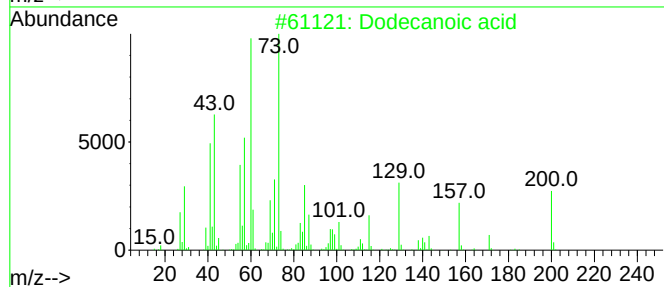
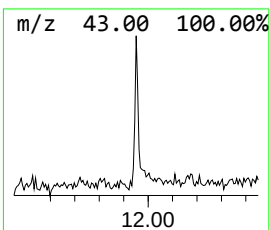
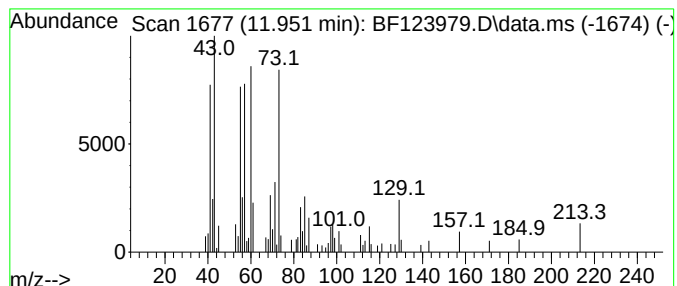
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Peak Number 2 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.77 ng	91844	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	80
2			Undecanoic acid	186	C11H22O2	000112-37-8	80
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	59
4			n-Decanoic acid	172	C10H20O2	000334-48-5	50
5			Trehalose	342	C12H22O11	000099-20-7	43



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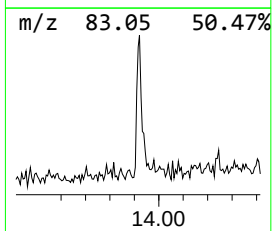
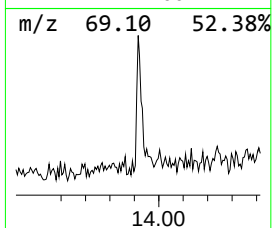
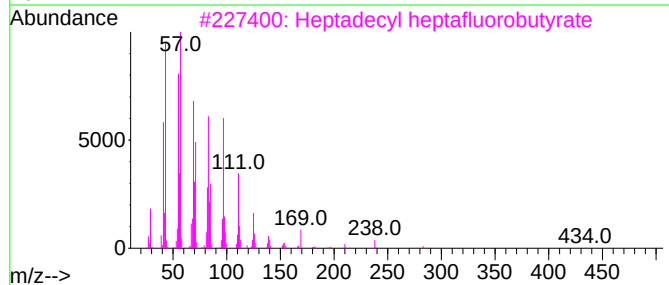
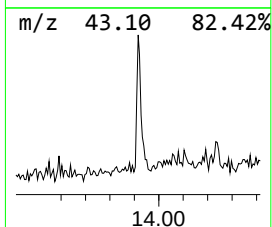
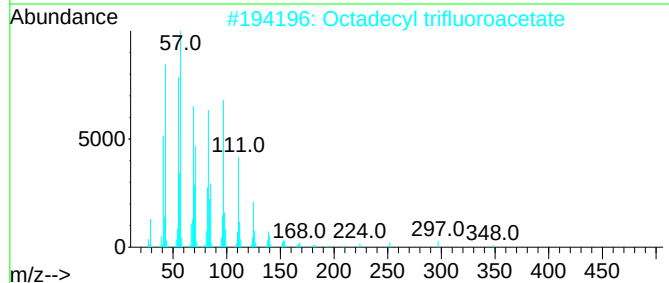
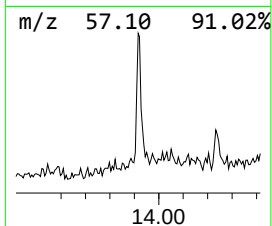
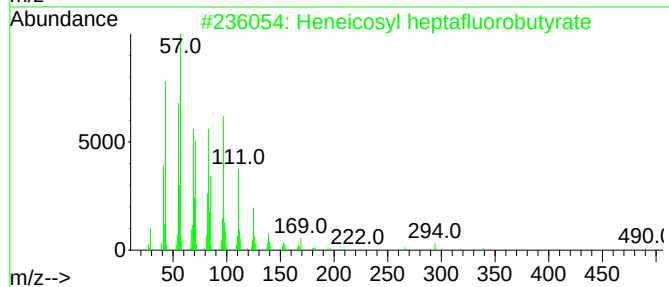
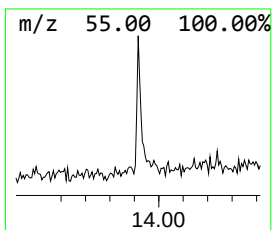
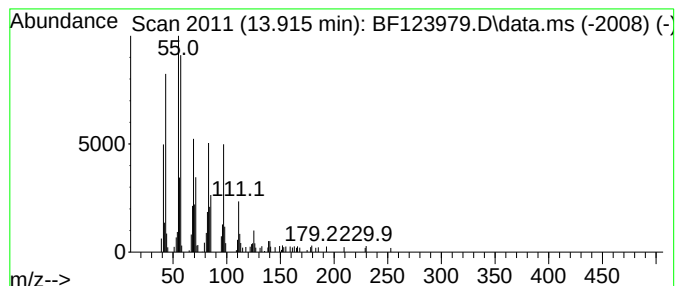
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Peak Number 3 Heneicosyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	12.73 ng	198127	Chrysene-d12	14.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
2			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
4			Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	91
5			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91



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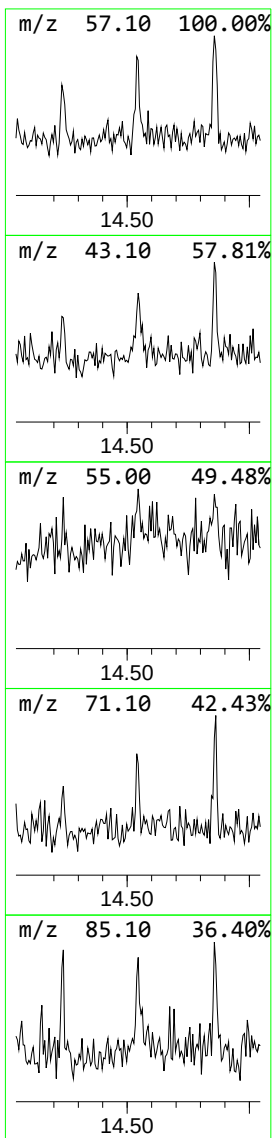
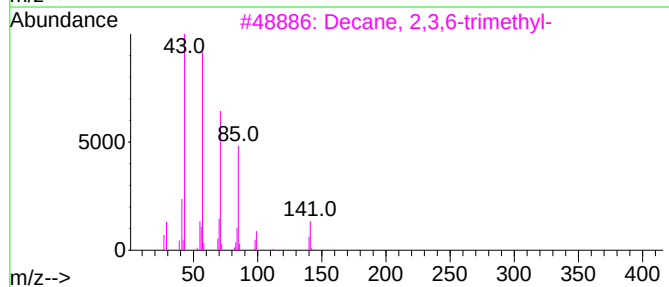
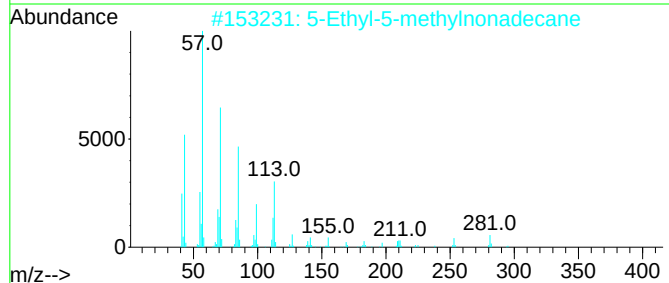
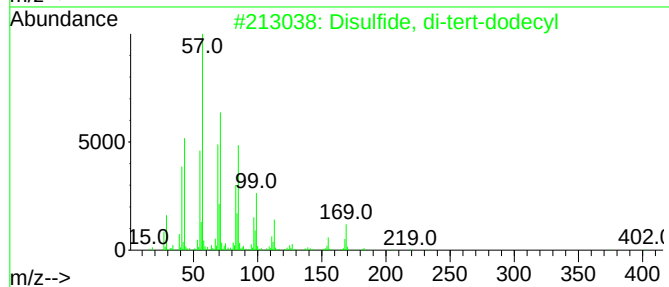
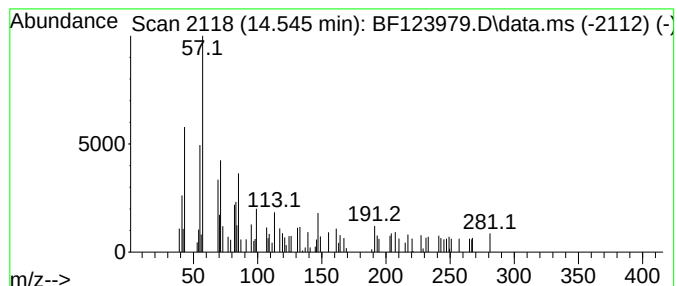
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Disulfide, di-tert-dodecyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.545	2.81 ng	43696	Chrysene-d12		14.074	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Disulfide, di-tert-dodecyl		402	C24H50S2	027458-90-8	52
2	5-Ethyl-5-methylnonadecane		310	C22H46	1000360-42-7	47
3	Decane, 2,3,6-trimethyl-		184	C13H28	062238-12-4	43
4	Hexane, 3,3-dimethyl-		114	C8H18	000563-16-6	43
5	Octadecane, 1-iodo-		380	C18H37I	000629-93-6	43



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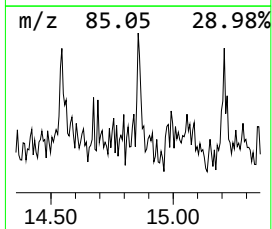
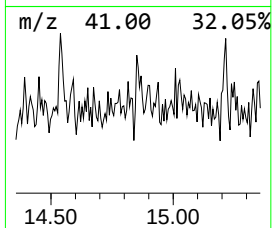
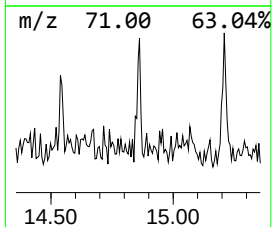
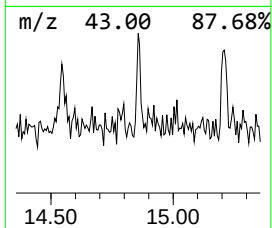
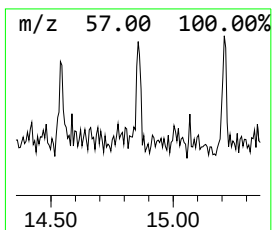
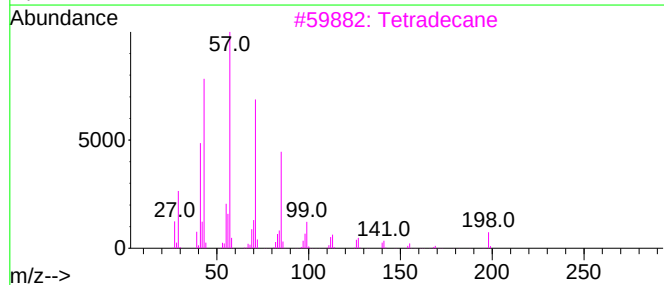
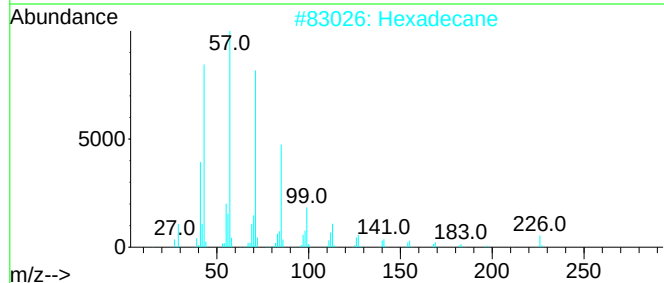
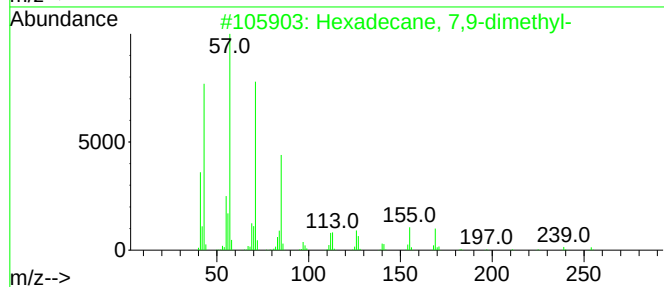
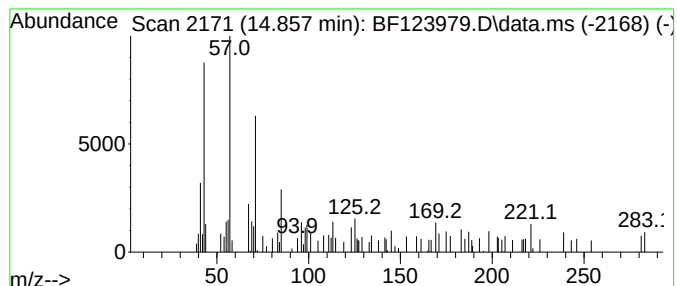
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Peak Number 5 Hexadecane, 7,9-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.857	2.56 ng	41730	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	55
2			Hexadecane	226	C16H34	000544-76-3	50
3			Tetradecane	198	C14H30	000629-59-4	50
4			Octadecane	254	C18H38	000593-45-3	49
5			5-Iodo-nonane	254	C9H19I	059456-19-8	46



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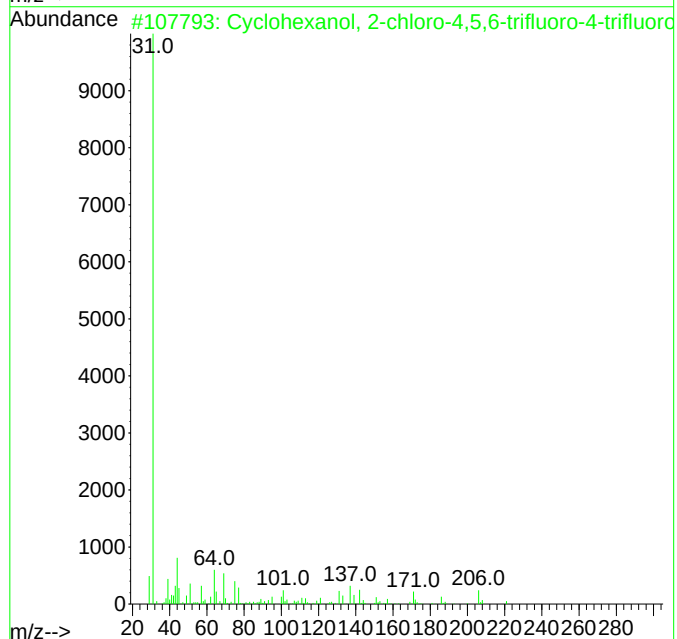
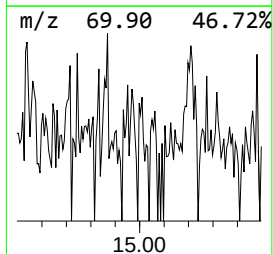
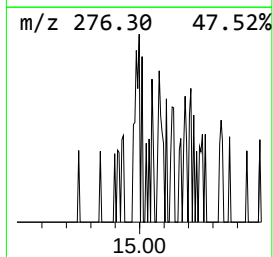
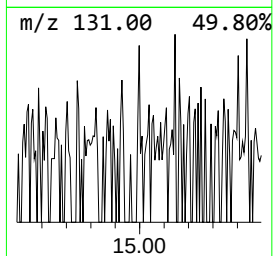
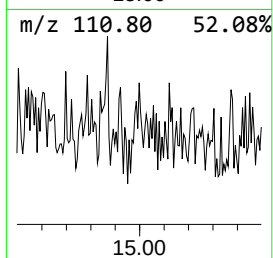
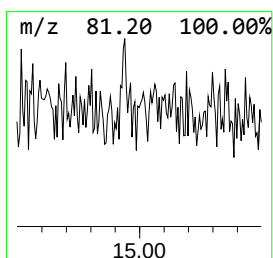
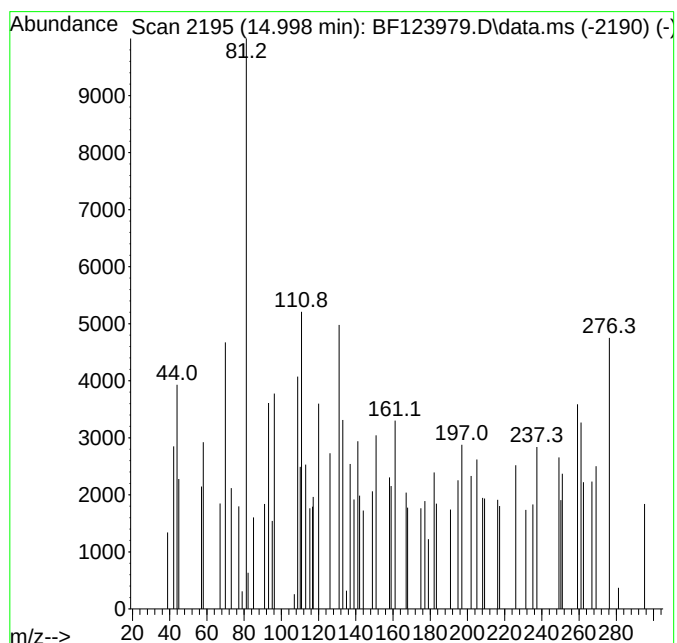
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Peak Number 6 unknown14.998 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.998	2.10 ng	34171	Perylene-d12	15.568
Hit# of	1	Tentative ID	MW MolForm	CAS# Qual
1	Cyclohexanol, 2-chloro-4,5,6-tri...	256	C7H7ClF6O	1000277-59-7 2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
Data File : BF123979.D
Acq On : 18 May 2021 15:25
Operator : JU/CG
Sample : M2435-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOMESTEAD-B

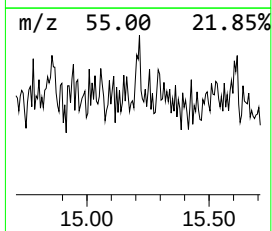
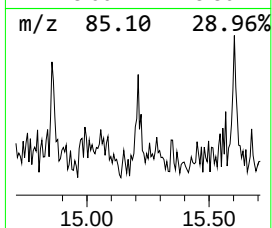
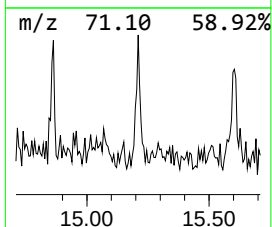
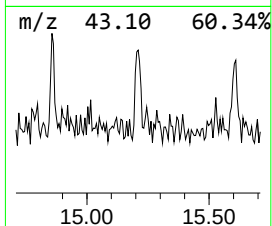
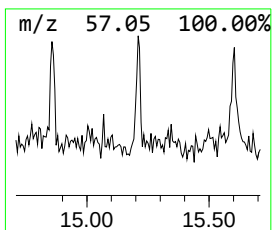
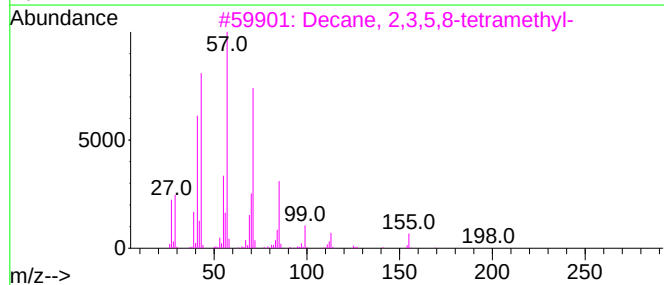
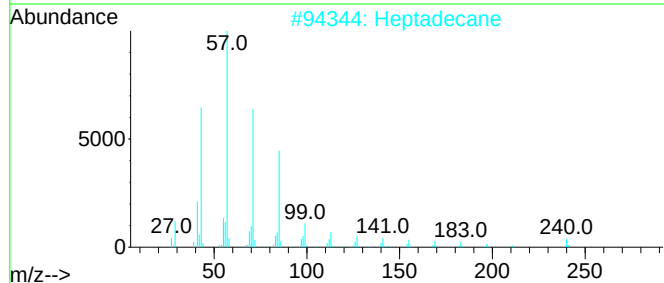
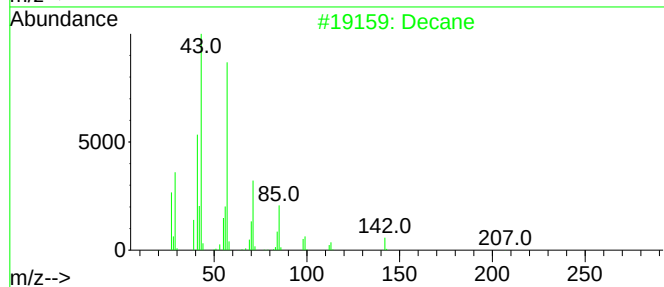
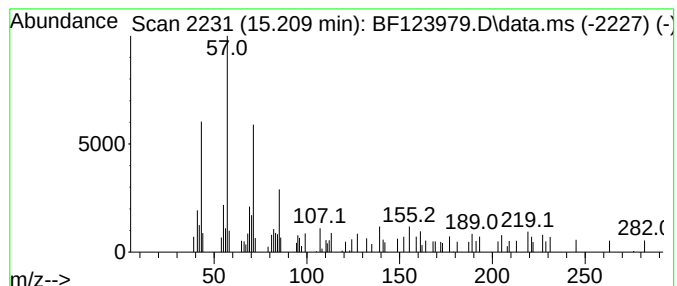
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.210 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.210	3.59 ng	58439	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane	142	C10H22	000124-18-5	43
2			Heptadecane	240	C17H36	000629-78-7	43
3			Decane, 2,3,5,8-tetramethyl-	198	C14H30	192823-15-7	43
4			Dodecane	170	C12H26	000112-40-3	38
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
Data File : BF123979.D
Acq On : 18 May 2021 15:25
Operator : JU/CG
Sample : M2435-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOMESTEAD-B

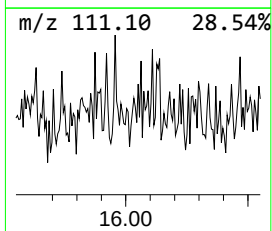
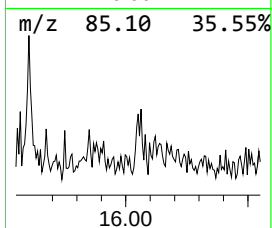
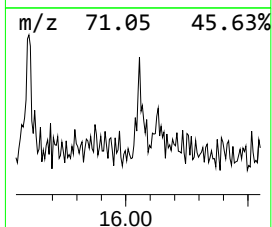
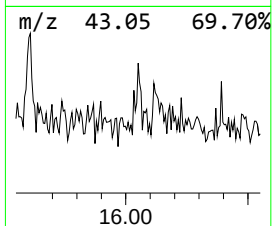
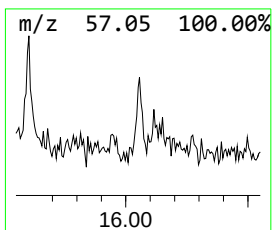
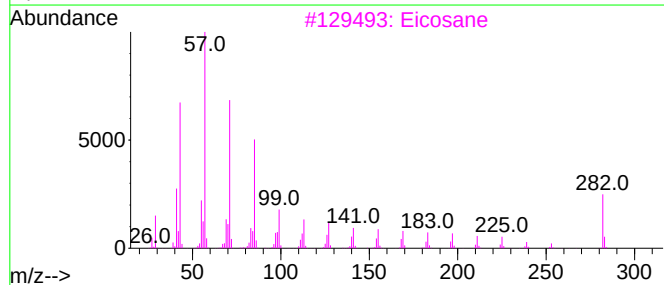
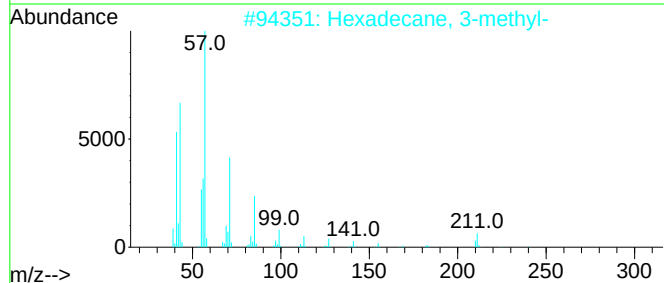
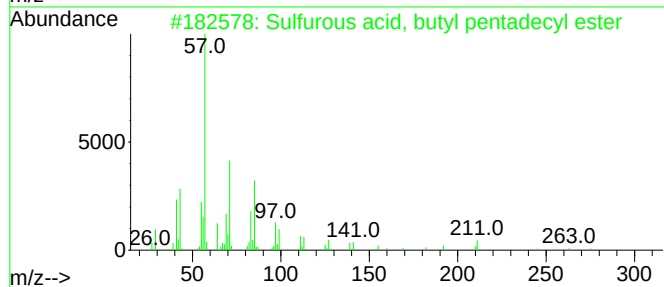
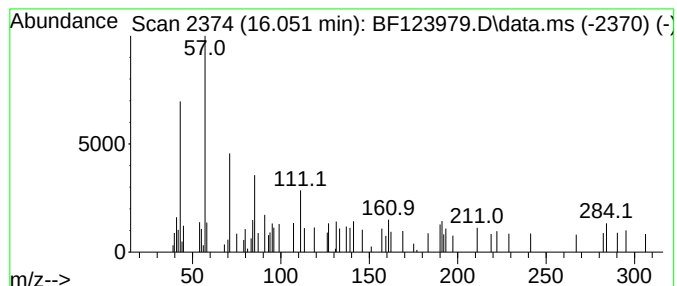
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.051 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.051	2.56 ng	41719	Perylene-d12	15.568

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	43
2			Hexadecane, 3-methyl-	240	C17H36	006418-43-5	38
3			Eicosane	282	C20H42	000112-95-8	38
4			Dotetracontane	591	C42H86	007098-20-6	35
5			Octadecane, 2-methyl-	268	C19H40	001560-88-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051821\
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Sample : M2435-10
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HOMESTEAD-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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...	2.199	50.9	ng	825981	1	6.904	324561	20.0
Dodecanoic acid	11.951	3.8	ng	91844	4	11.427	487652	20.0
Heneicosyl hept...	13.915	12.7	ng	198127	5	14.074	311394	20.0
Disulfide, di-t...	14.545	2.8	ng	43696	5	14.074	311394	20.0
Hexadecane, 7,9...	14.857	2.6	ng	41730	6	15.568	325913	20.0
unknown14.998	14.998	2.1	ng	34171	6	15.568	325913	20.0
unknown15.210	15.210	3.6	ng	58439	6	15.568	325913	20.0
unknown16.051	16.051	2.6	ng	41719	6	15.568	325913	20.0