

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
 Data File : BF122365.D
 Acq On : 18 Nov 2020 13:53
 Operator : JU/CG
 Sample : L4770-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FJ-BH-03-4-5

Integration Parameters: rteint.p

Integrator: RTE

Smothing : 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-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.128	3	7	33	rVB	746946	1265243	20.74%	3.044%
2	2.299	34	36	51	rVB2	63385	113272	1.86%	0.272%
3	5.063	502	506	513	rVB	316172	354485	5.81%	0.853%
4	5.469	571	575	579	rBV	3227120	2965532	48.60%	7.134%
5	6.481	742	747	750	rBV	3976172	3561851	58.38%	8.568%
6	6.863	809	812	815	rBV	1806612	1353868	22.19%	3.257%
7	7.422	903	907	910	rBV	2905888	2485404	40.73%	5.979%
8	8.145	1027	1030	1034	rBV	1965926	1786558	29.28%	4.298%
9	9.228	1209	1214	1217	rBV	5149027	4828257	79.13%	11.614%
10	9.616	1276	1280	1290	rVB	944482	752788	12.34%	1.811%
11	9.904	1325	1329	1340	rVB	2613731	2185775	35.82%	5.258%
12	10.686	1458	1462	1472	rBV	2167250	2044864	33.51%	4.919%
13	11.386	1577	1581	1585	rBV	2662053	2322194	38.06%	5.586%
14	11.916	1667	1671	1681	rBV3	193869	348427	5.71%	0.838%
15	12.374	1745	1749	1752	rBV	308718	291659	4.78%	0.702%
16	12.427	1755	1758	1762	rVB	75314	66847	1.10%	0.161%
17	12.639	1788	1794	1798	rBV9	30960	74273	1.22%	0.179%
18	12.704	1800	1805	1815	rVV	775504	1190950	19.52%	2.865%
19	12.974	1847	1851	1855	rBV	6315304	6101547	100.00%	14.677%
20	13.880	2001	2005	2023	rBV	582867	1224734	20.07%	2.946%
21	14.027	2025	2030	2033	rBV	2773854	2513166	41.19%	6.045%
22	14.198	2056	2059	2069	rVB3	81752	192411	3.15%	0.463%
23	14.504	2106	2111	2113	rBV2	73598	77386	1.27%	0.186%
24	14.533	2113	2116	2125	rVV2	31872	77346	1.27%	0.186%
25	14.662	2133	2138	2143	rBV	163072	283894	4.65%	0.683%
26	14.810	2161	2163	2168	rVB	79527	92997	1.52%	0.224%
27	14.886	2173	2176	2182	rVB2	72359	90167	1.48%	0.217%
28	15.157	2218	2222	2225	rBV	70516	80202	1.31%	0.193%
29	15.498	2274	2280	2284	rBV	1958752	2360810	38.69%	5.679%
30	15.539	2284	2287	2292	rVB2	64301	86868	1.42%	0.209%
31	15.980	2358	2362	2366	rVB	48326	66355	1.09%	0.160%
32	18.339	2751	2763	2774	rVB9	73939	331710	5.44%	0.798%

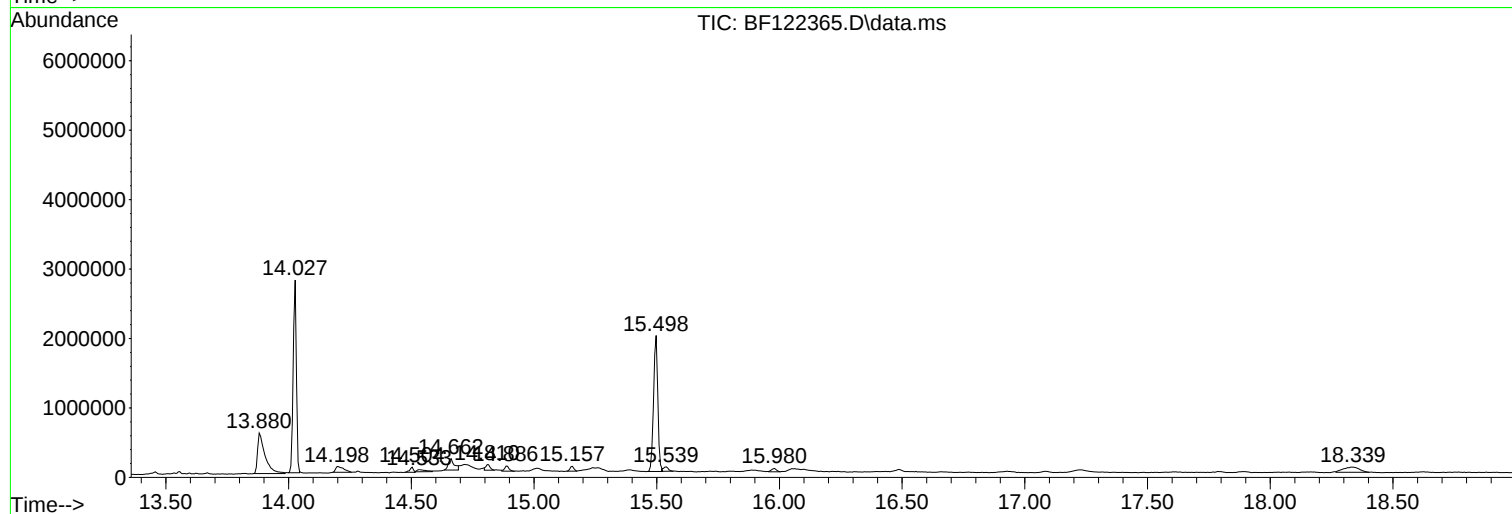
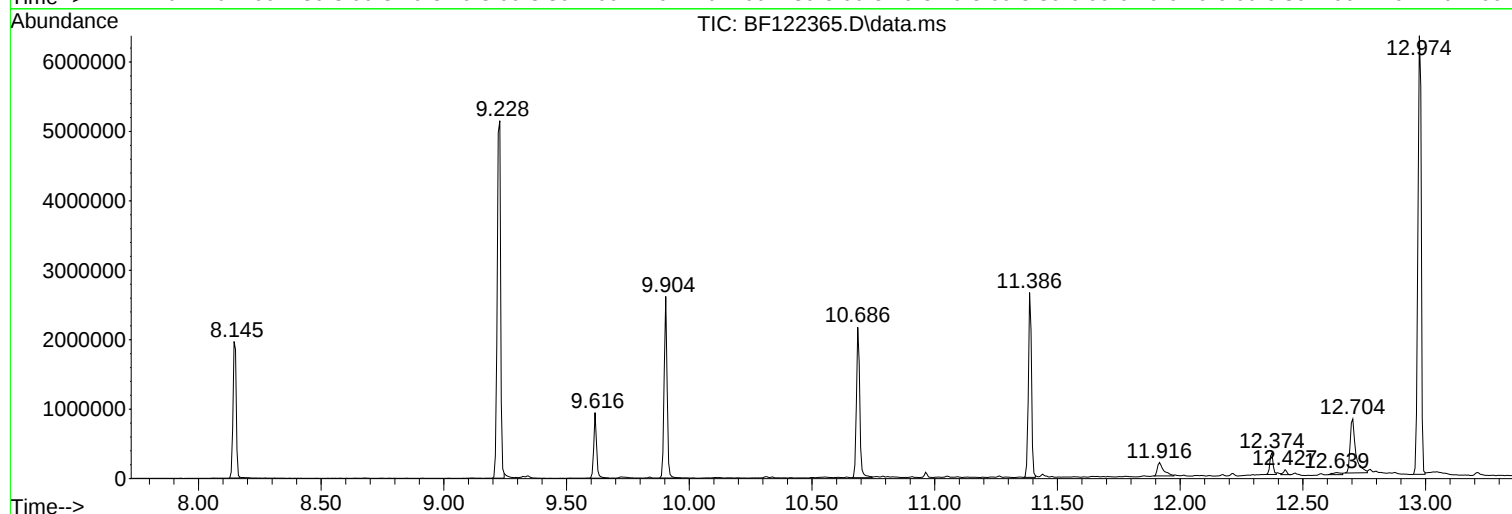
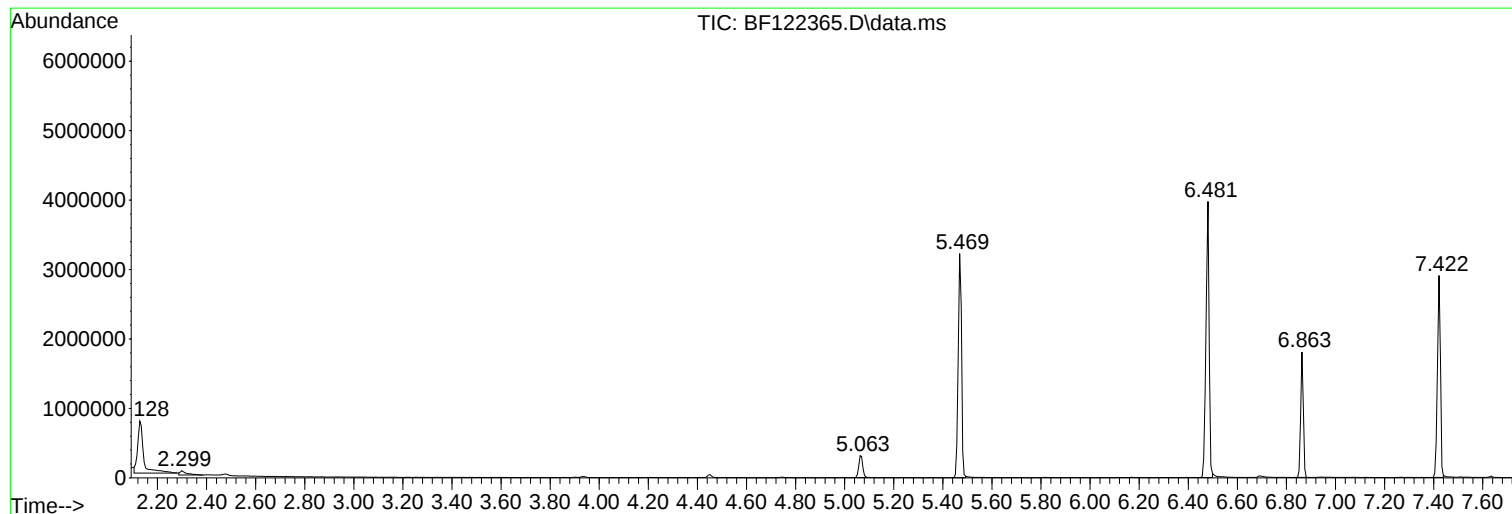
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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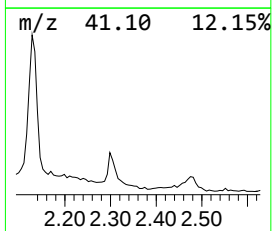
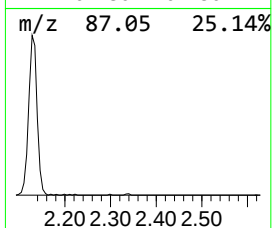
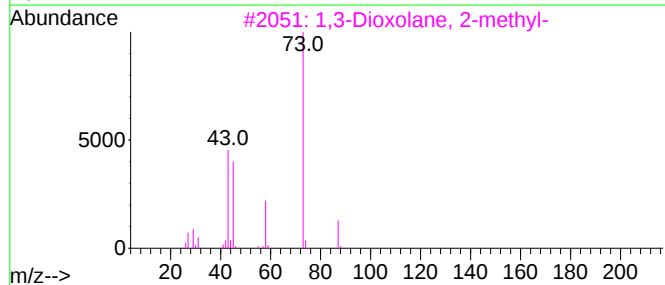
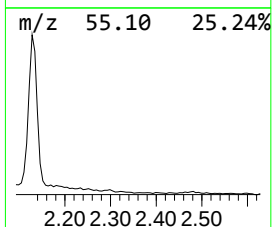
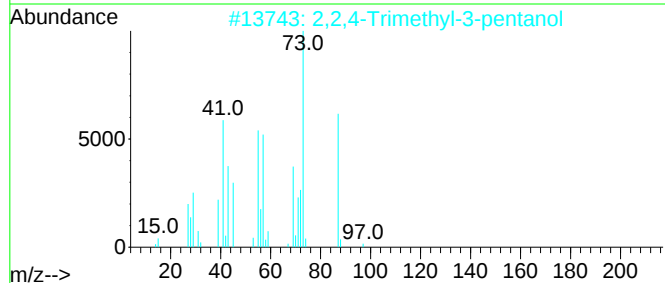
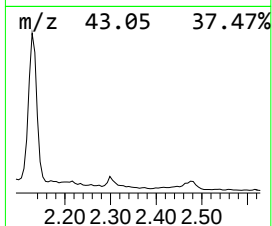
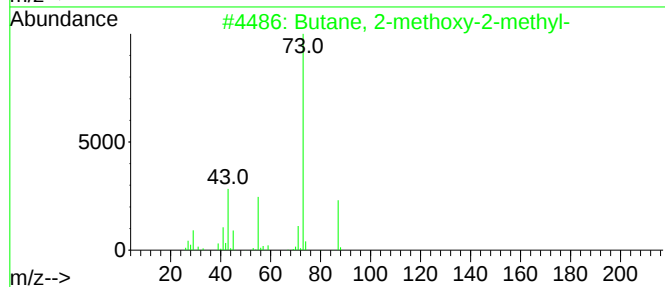
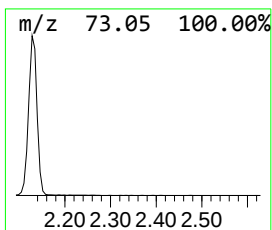
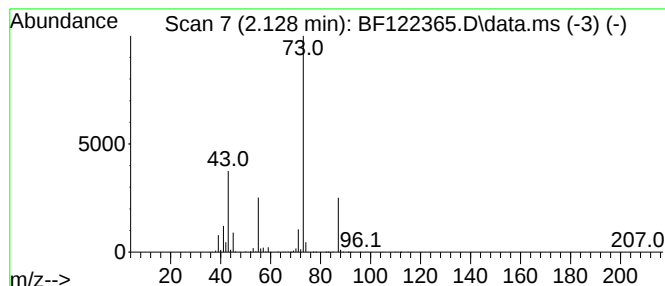
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.128	18.69 ng	1265240	1,4-Dichlorobenzene-d4	6.863

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			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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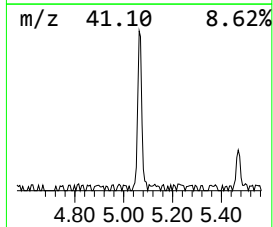
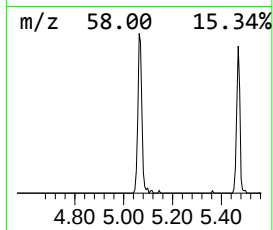
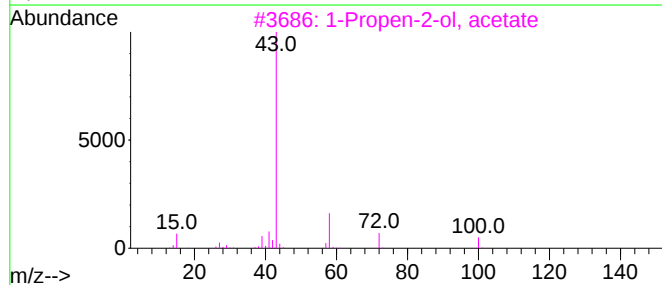
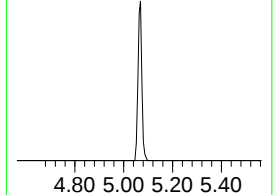
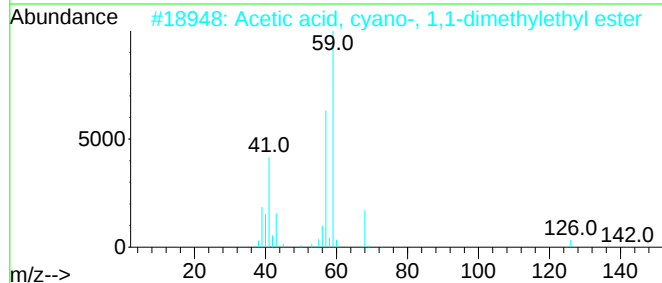
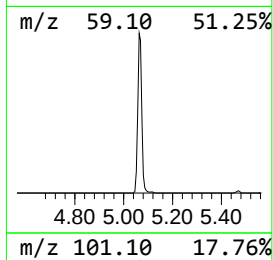
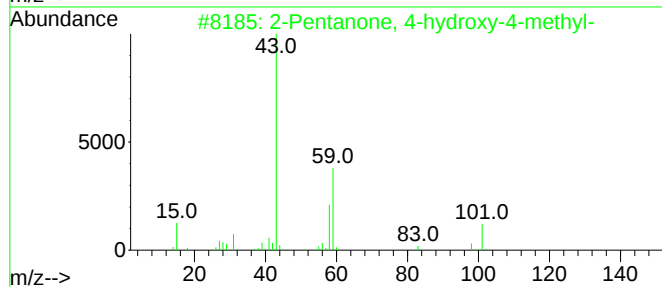
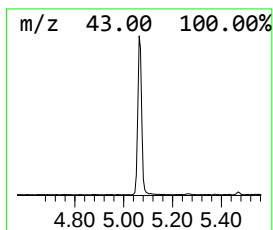
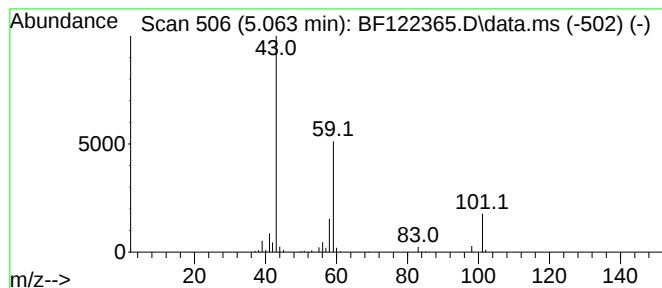
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	5.24 ng	354485	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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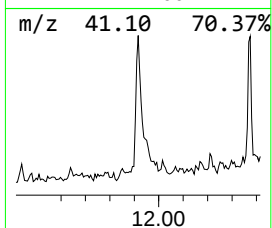
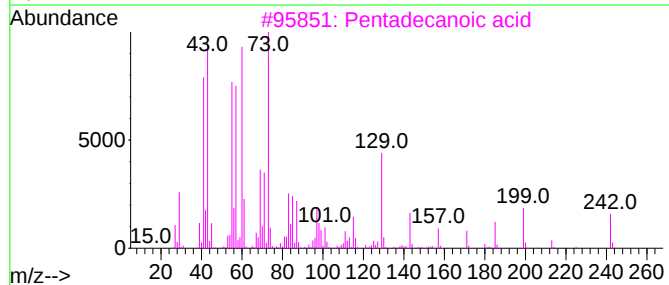
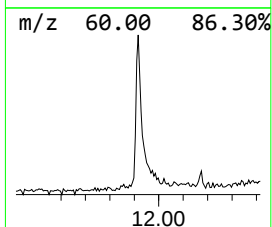
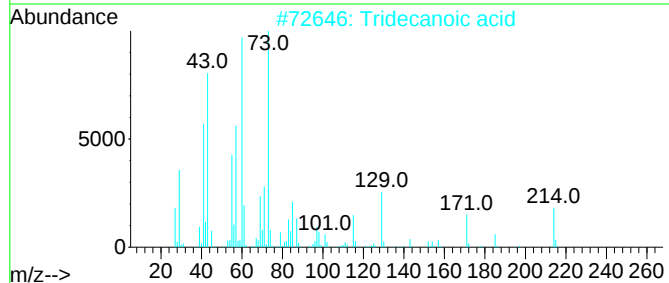
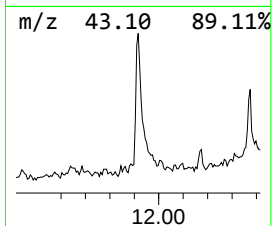
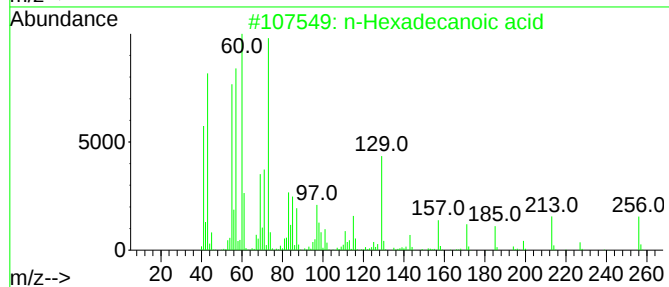
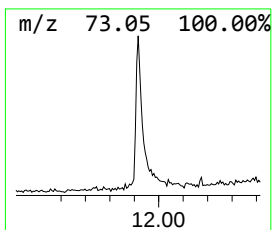
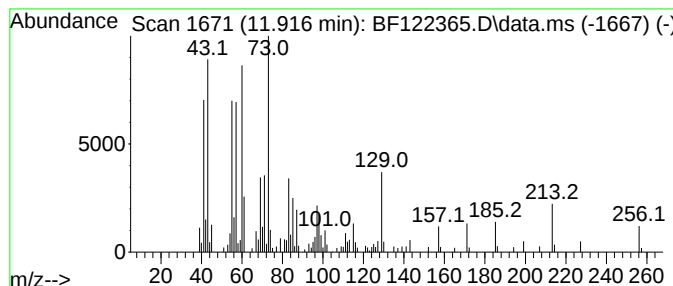
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	3.00 ng	348427	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	76
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4			Undecanoic acid	186	C11H22O2	000112-37-8	59
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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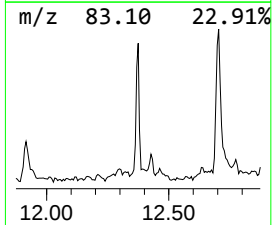
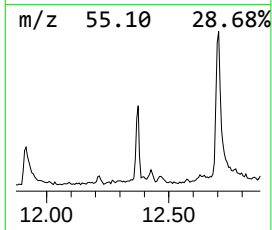
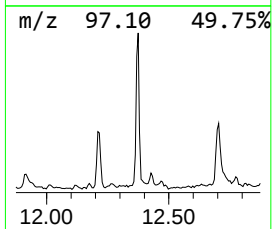
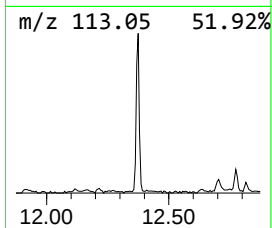
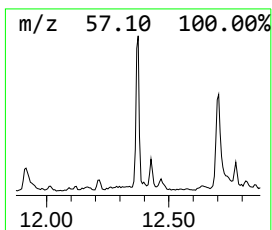
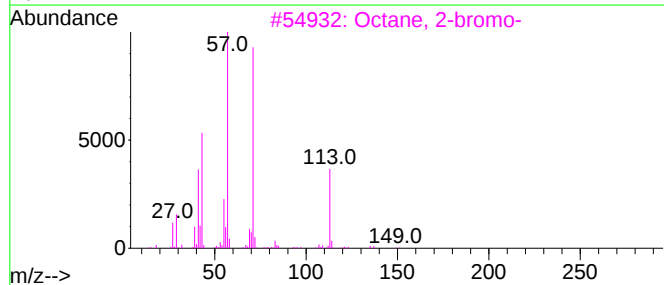
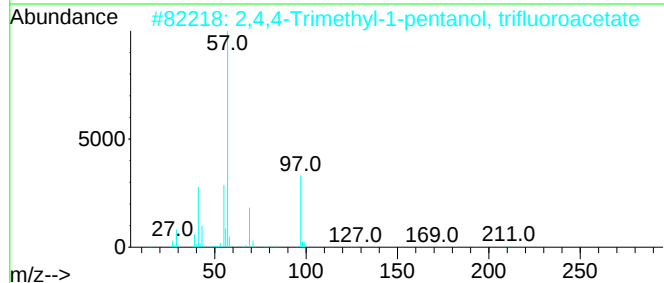
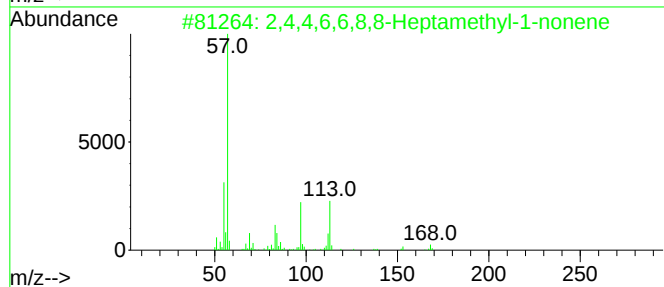
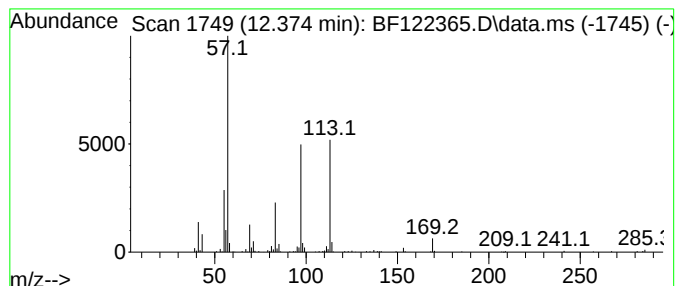
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown12.37 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.374	2.51 ng	291659	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			2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	35
3			Octane, 2-bromo-	192	C8H17Br	000557-35-7	25
4			Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25
5			2,2-Dimethyl-3-pentanol, heptafl...	312	C11H15F7O2	1000364-14-4	22



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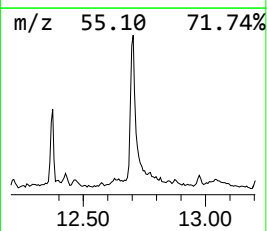
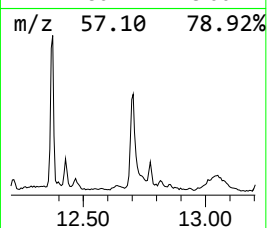
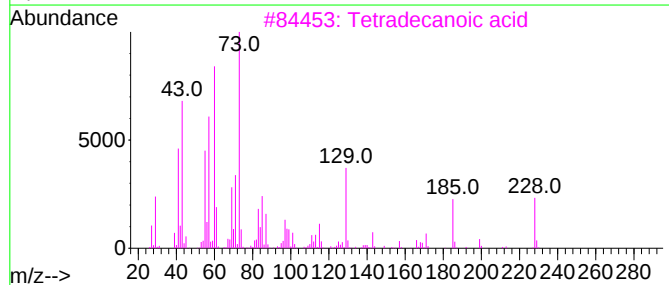
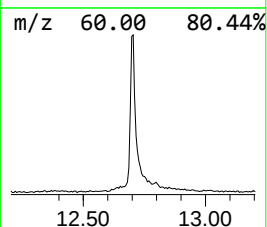
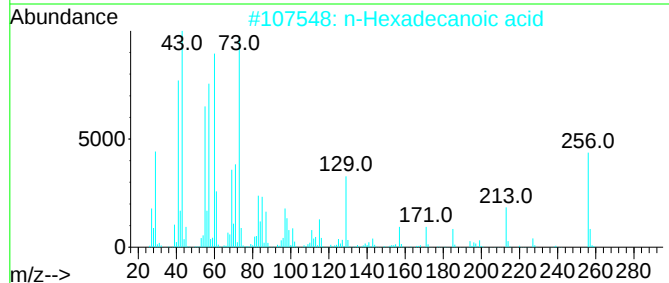
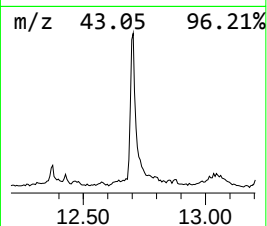
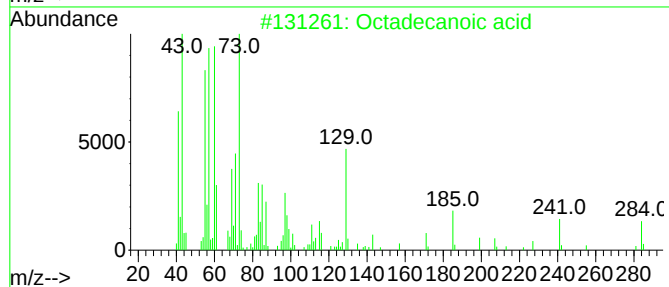
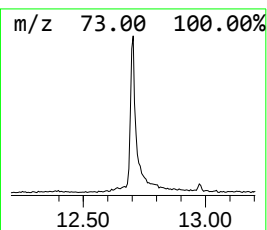
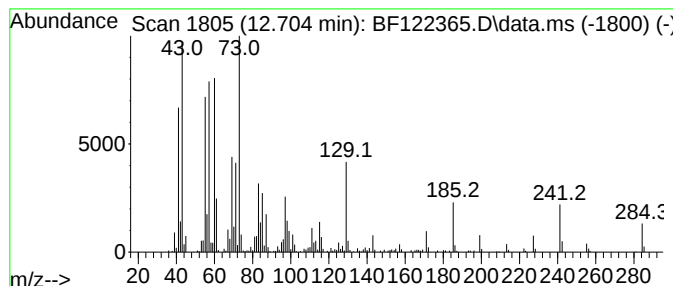
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.704	10.26 ng	1190950	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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FJ-BH-03-4-5

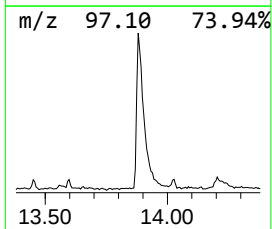
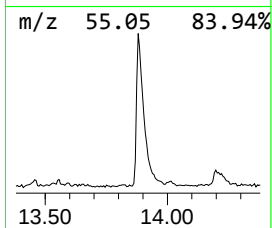
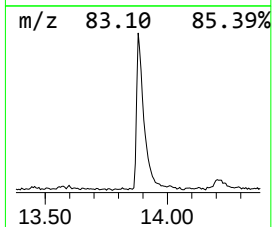
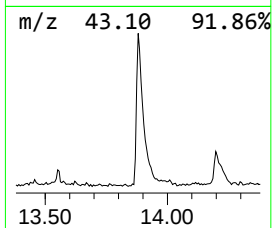
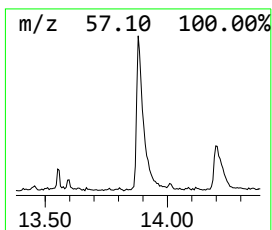
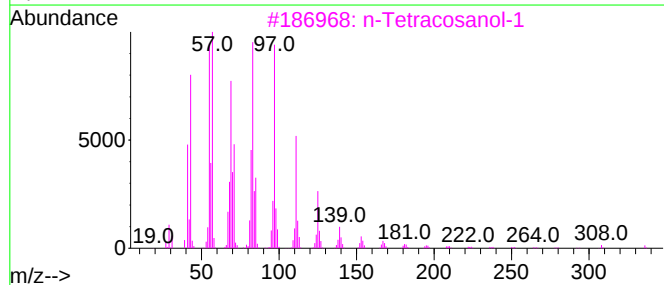
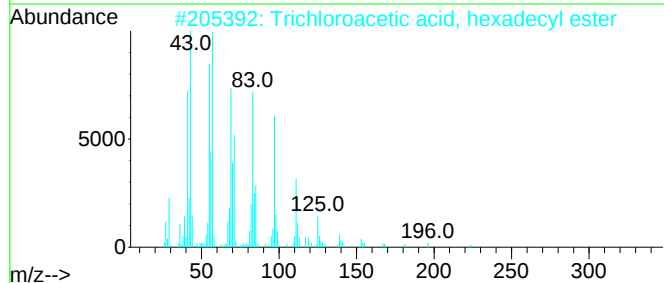
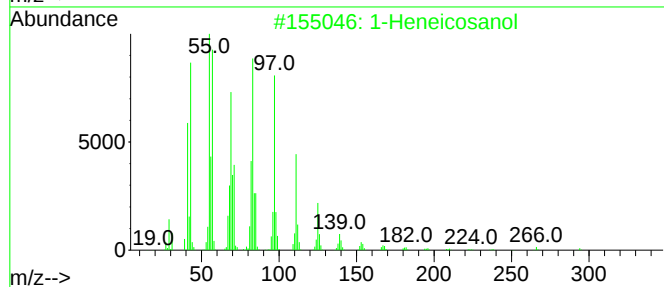
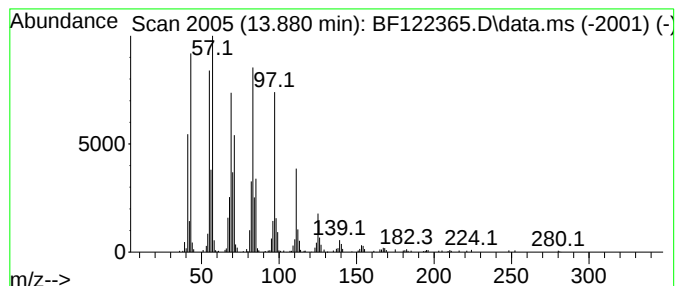
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	9.75 ng	1224730	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122365.D
Acq On : 18 Nov 2020 13:53
Operator : JU/CG
Sample : L4770-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FJ-BH-03-4-5

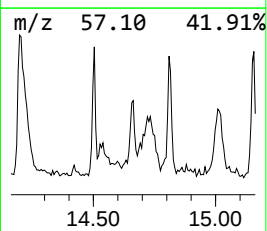
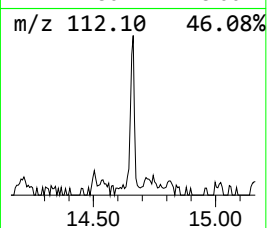
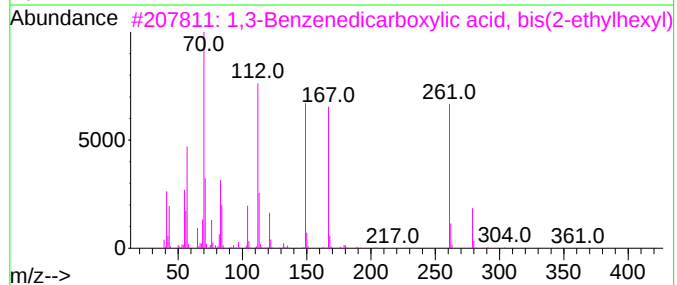
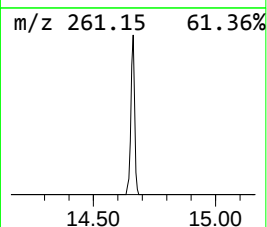
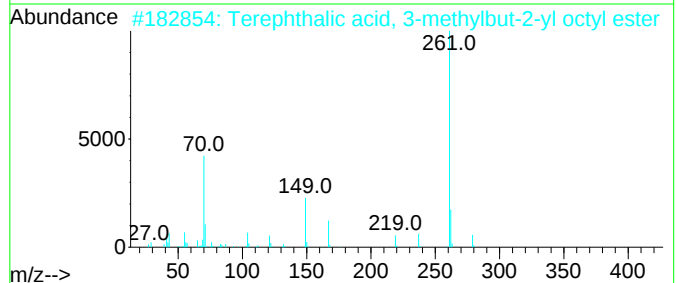
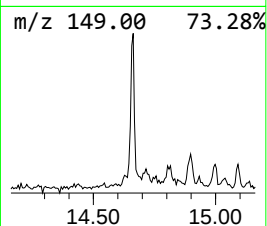
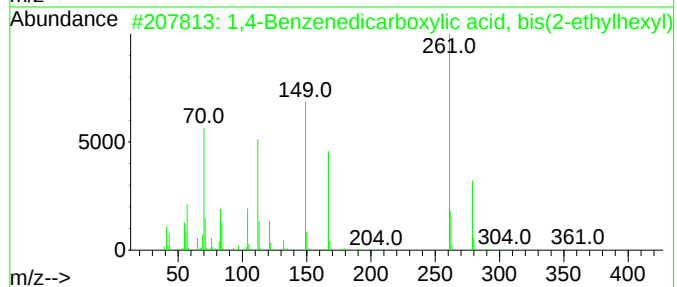
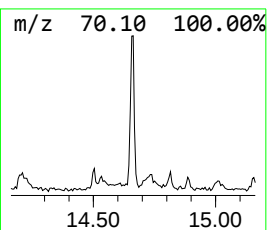
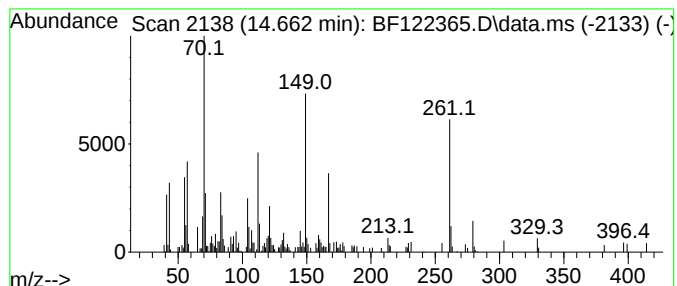
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.663	2.26 ng	283894	Chrysene-d12	14.027

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	74
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	43
4			Terephthalic acid, 3,4-dimethylp...	382	C24H30O4	1000323-67-4	35
5			Phthalic acid, 3,5-difluoropheny...	390	C22H24F2O4	1000315-51-3	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122365.D
Acq On : 18 Nov 2020 13:53
Operator : JU/CG
Sample : L4770-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FJ-BH-03-4-5

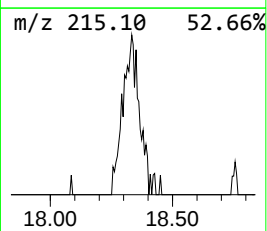
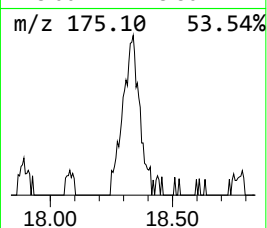
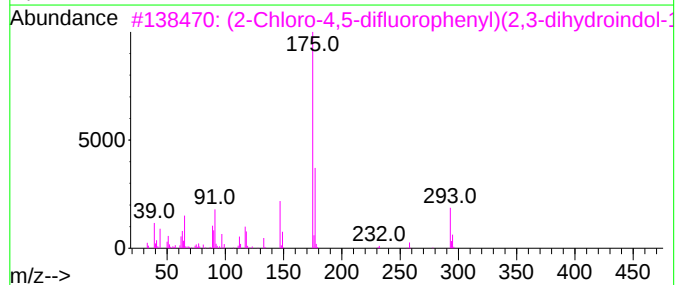
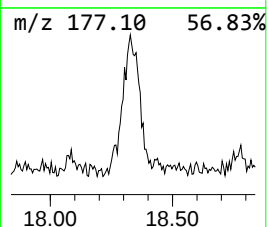
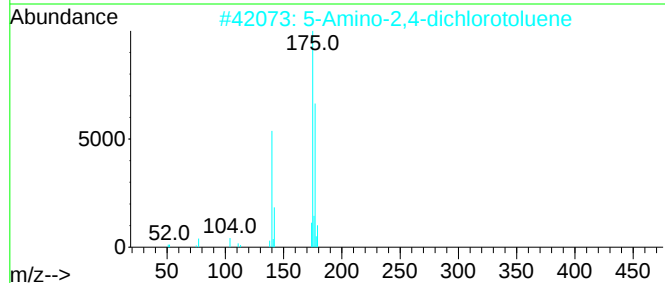
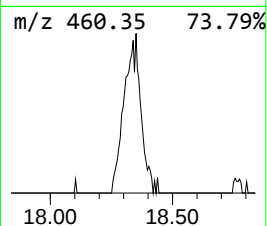
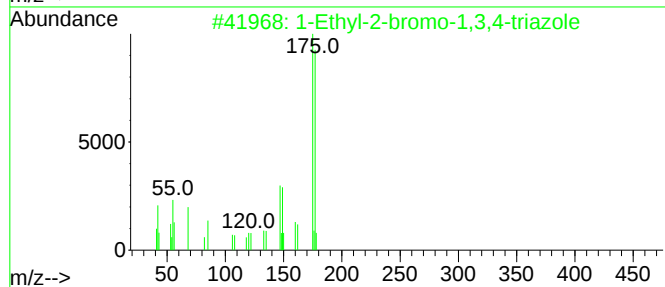
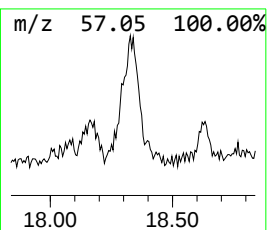
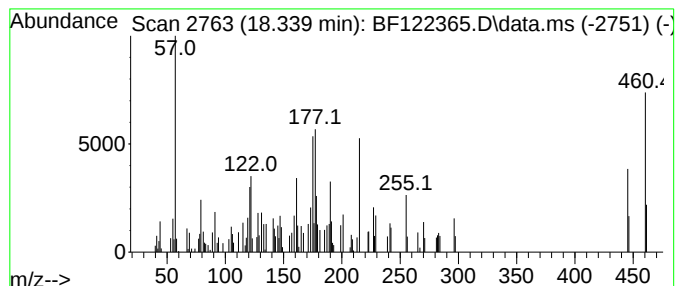
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.33 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.339	2.81 ng	331710	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Ethyl-2-bromo-1,3,4-triazole	175	C4H6BrN3	064907-56-8	10
2			5-Amino-2,4-dichlorotoluene	175	C7H7Cl2N	017601-75-1	9
3			(2-Chloro-4,5-difluorophenyl)(2,...	293	C15H10ClF2NO	1000317-20-2	9
4			Silane, dichloromethylphenyl-	190	C7H8Cl2Si	000149-74-6	9
5			Silane, tert-butyldichlorophenyl-	232	C10H14Cl2Si	017887-41-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111820\
Data File : BF122365.D
Acq On : 18 Nov 2020 13:53
Operator : JU/CG
Sample : L4770-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
FJ-BH-03-4-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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...	2.128	18.7	ng	1265240	1	6.863	1353870	20.0
2-Pentanone, 4-...	5.063	5.2	ng	354485	1	6.863	1353870	20.0
n-Hexadecanoic ...	11.916	3.0	ng	348427	4	11.386	2322190	20.0
unknown12.37	12.374	2.5	ng	291659	4	11.386	2322190	20.0
Octadecanoic acid	12.704	10.3	ng	1190950	4	11.386	2322190	20.0
1-Heneicosanol	13.880	9.8	ng	1224730	5	14.027	2513170	20.0
1,4-Benzenedica...	14.663	2.3	ng	283894	5	14.027	2513170	20.0
unknown18.33	18.339	2.8	ng	331710	6	15.498	2360810	20.0