

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
 Data File : BG049974.D
 Acq On : 25 Aug 2021 18:59
 Operator : CG/JU
 Sample : M3530-01 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PL-01-082421

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_G\Methods\8270-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049974.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.067	3	5	14	rVB2	20681	30355	4.35%	0.494%
2	5.540	418	426	433	rBV	83484	146630	21.03%	2.385%
3	7.155	694	701	709	rBV2	87973	165504	23.74%	2.692%
4	7.978	835	841	850	rBV	117738	205929	29.53%	3.350%
5	9.152	1034	1041	1054	rVB2	60391	114033	16.35%	1.855%
6	10.568	1276	1282	1292	rVB4	13360	28506	4.09%	0.464%
7	10.803	1315	1322	1328	rBV	159936	288871	41.43%	4.699%
8	12.466	1599	1605	1610	rVB3	7586	13479	1.93%	0.219%
9	12.689	1638	1643	1646	rBV	4922	7015	1.01%	0.114%
10	13.253	1733	1739	1746	rVB	156208	235438	33.76%	3.830%
11	13.441	1766	1771	1774	rBV4	4806	8888	1.27%	0.145%
12	13.958	1855	1859	1865	rVB7	5004	7655	1.10%	0.125%
13	14.369	1923	1929	1932	rBV3	5339	10376	1.49%	0.169%
14	14.516	1950	1954	1958	rBV5	8318	11759	1.69%	0.191%
15	14.639	1967	1975	1981	rBV	238353	367765	52.74%	5.982%
16	14.698	1981	1985	1991	rVB2	10557	16332	2.34%	0.266%
17	15.033	2038	2042	2051	rVB4	12263	23807	3.41%	0.387%
18	15.467	2113	2116	2119	rVB3	14144	16406	2.35%	0.267%
19	15.691	2149	2154	2159	rBV2	17954	30257	4.34%	0.492%
20	15.867	2176	2184	2186	rBV6	8199	18840	2.70%	0.306%
21	16.137	2220	2230	2237	rVB	116006	192163	27.56%	3.126%
22	16.331	2259	2263	2266	rBV5	19897	31170	4.47%	0.507%
23	16.742	2330	2333	2337	rVB6	6834	8857	1.27%	0.144%
24	16.848	2345	2351	2352	rVB5	6125	8559	1.23%	0.139%
25	17.130	2393	2399	2403	rBV4	24396	38369	5.50%	0.624%
26	17.183	2403	2408	2410	rBV4	11573	16288	2.34%	0.265%
27	17.394	2436	2444	2448	rBV	249950	402596	57.74%	6.548%
28	17.435	2448	2451	2459	rVV	128750	178625	25.62%	2.905%
29	17.523	2460	2466	2471	rVV	32583	50571	7.25%	0.823%
30	17.800	2509	2513	2518	rVB6	8113	12301	1.76%	0.200%
31	17.864	2521	2524	2528	rVB2	17218	21777	3.12%	0.354%
32	17.911	2528	2532	2537	rBV8	21876	26321	3.77%	0.428%
33	18.040	2549	2554	2560	rVB	174841	229308	32.89%	3.730%
34	18.270	2589	2593	2598	rBV2	21954	37976	5.45%	0.618%
35	18.322	2598	2602	2607	rVB2	29344	45683	6.55%	0.743%
36	18.399	2613	2615	2619	rBV4	10055	14170	2.03%	0.230%

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Instrument :
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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_G\Methods\8270-BG080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.469	2621	2627	2631	rBV3	36047	75341	10.80%	1.225%
38	18.563	2639	2643	2645	rBV3	16330	20349	2.92%	0.331%
39	18.763	2674	2677	2682	rBV2	16769	27438	3.93%	0.446%
40	18.810	2683	2685	2691	rVB7	9120	13544	1.94%	0.220%
41	19.098	2732	2734	2737	rBV4	8706	10923	1.57%	0.178%
42	19.180	2743	2748	2751	rBV	422109	568444	81.52%	9.246%
43	19.215	2751	2754	2758	rVB	606669	697287	100.00%	11.342%
44	19.345	2772	2776	2781	rVB	108712	134343	19.27%	2.185%
45	19.450	2789	2794	2799	rVB	208488	289125	41.46%	4.703%
46	19.779	2845	2850	2851	rBV2	36452	57187	8.20%	0.930%
47	19.809	2851	2855	2864	rVB	188434	283276	40.63%	4.608%
48	19.873	2864	2866	2869	rBV4	13009	18146	2.60%	0.295%
49	20.002	2883	2888	2893	rBV	189399	262421	37.63%	4.268%
50	20.402	2953	2956	2960	rVB3	29277	36113	5.18%	0.587%
51	21.665	3165	3171	3177	rBV3	214622	464354	66.59%	7.553%
52	21.718	3177	3180	3186	rVB	86749	127079	18.22%	2.067%

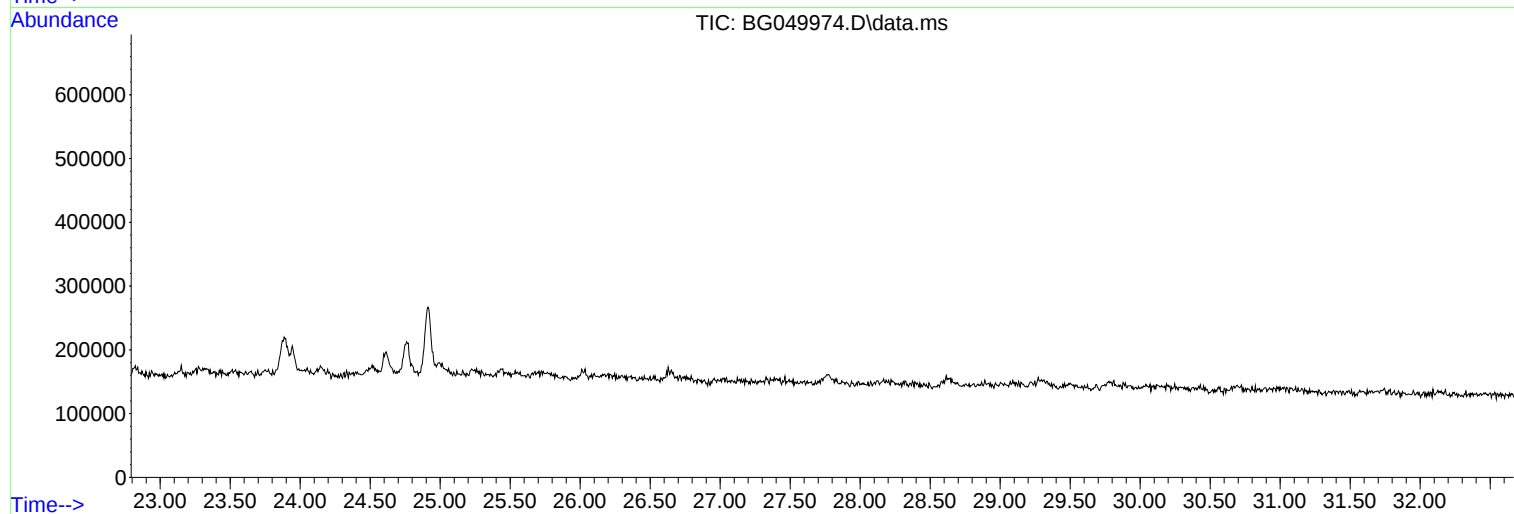
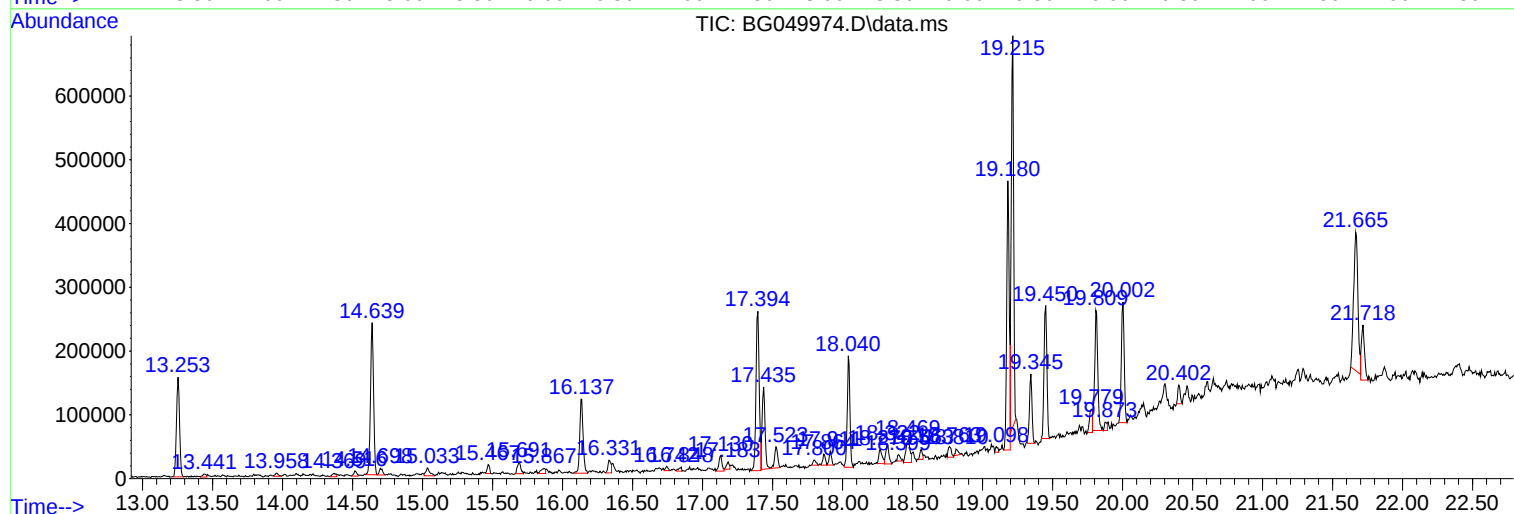
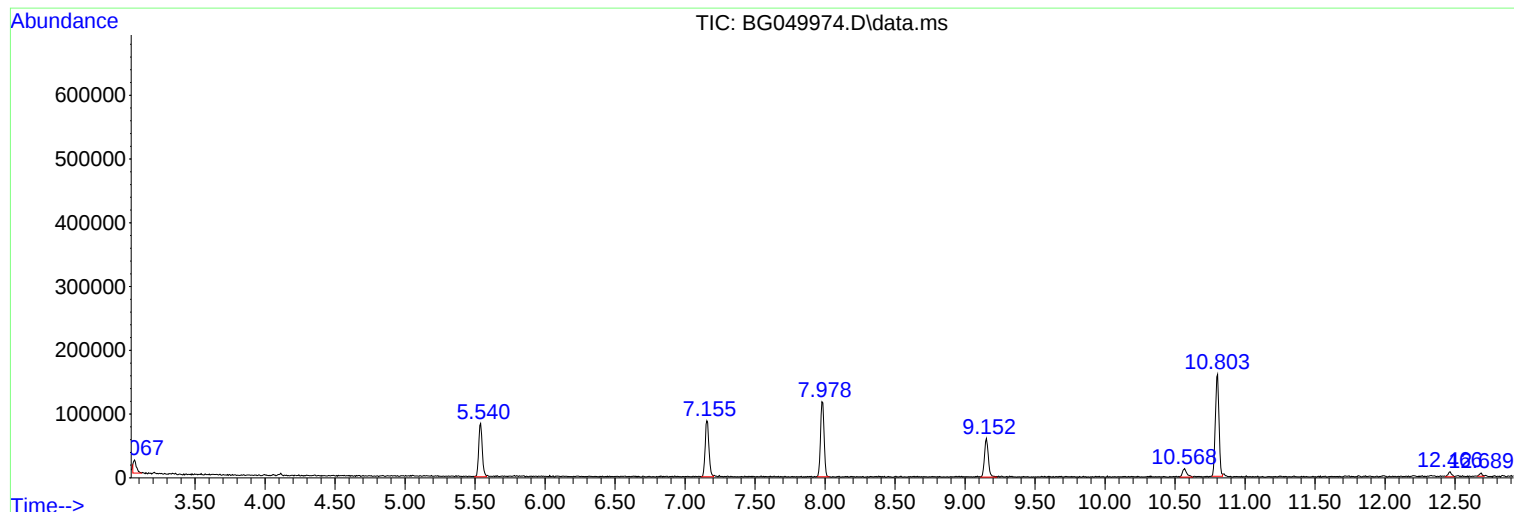
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : M3530-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PL-01-082421

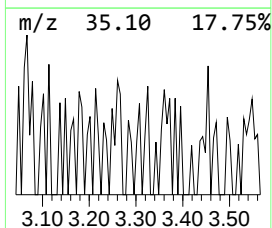
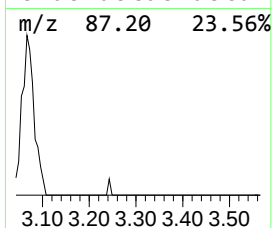
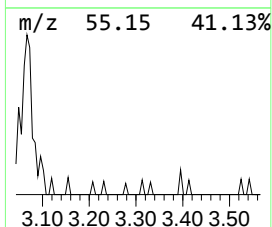
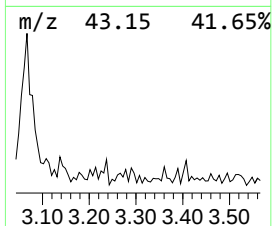
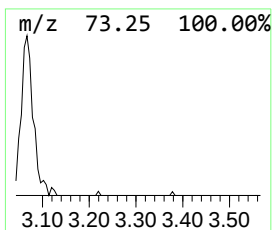
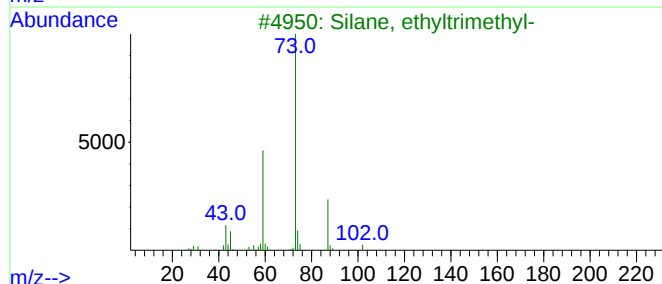
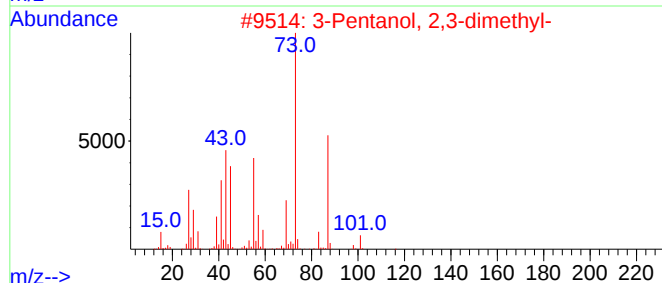
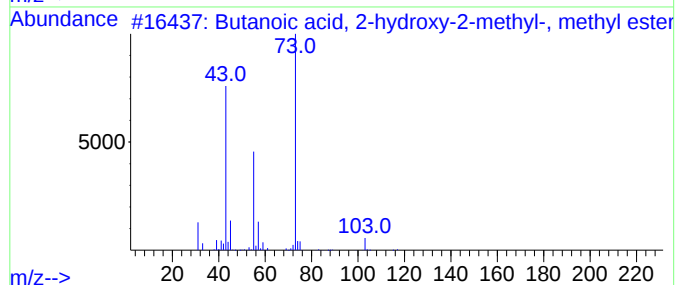
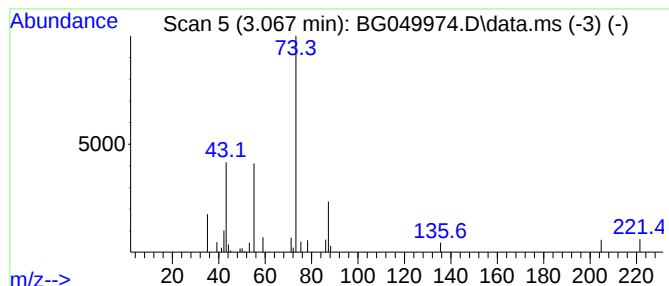
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.067 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.067	2.95 ng	30355	1,4-Dichlorobenzene-d4	7.978

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	12
2			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	9
3			Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9
4			Urea, butyl-	116	C5H12N2O	000592-31-4	9
5			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9



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Misc :
ALS Vial : 13 Sample Multiplier: 1

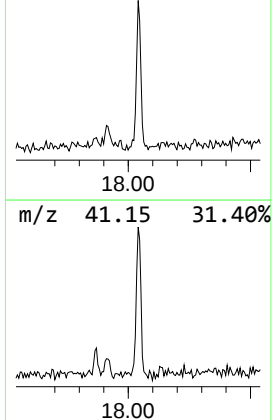
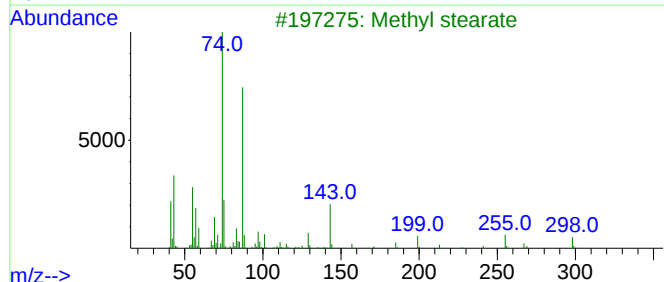
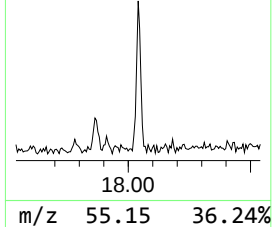
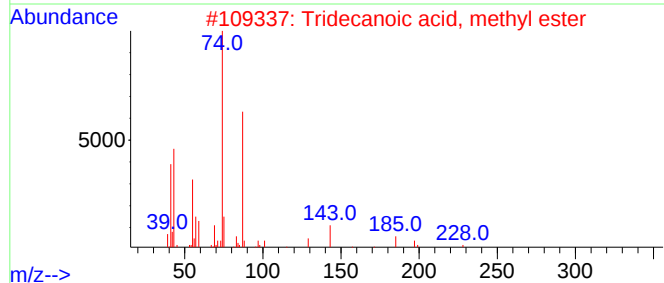
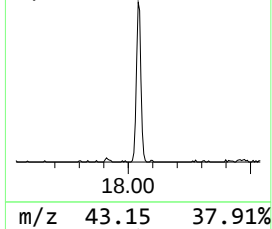
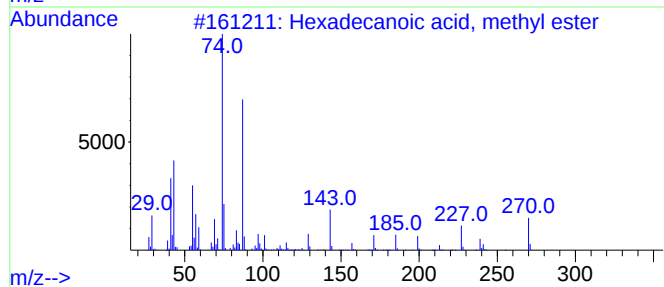
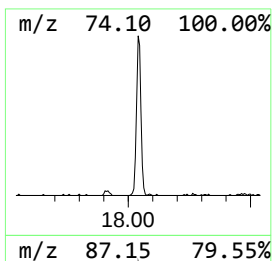
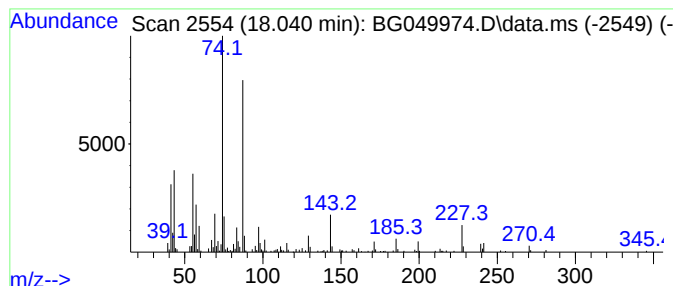
Instrument :
BNA_G
ClientSampleId :
PL-01-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.040	11.39 ng	229308	Phenanthrene-d10		17.394	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	94
2	Tridecanoic acid, methyl ester		228	C14H28O2	001731-88-0	87
3	Methyl stearate		298	C19H38O2	000112-61-8	86
4	Tridecanoic acid, 12-methyl-, me...		242	C15H30O2	005129-58-8	80
5	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	80



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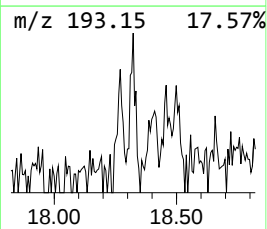
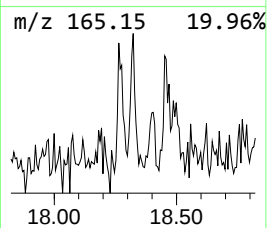
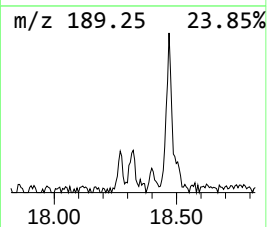
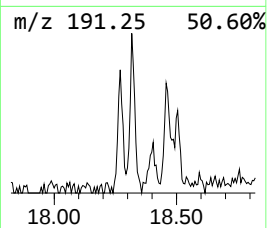
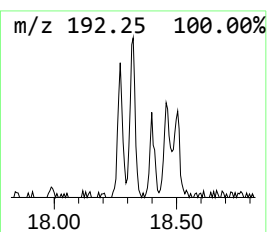
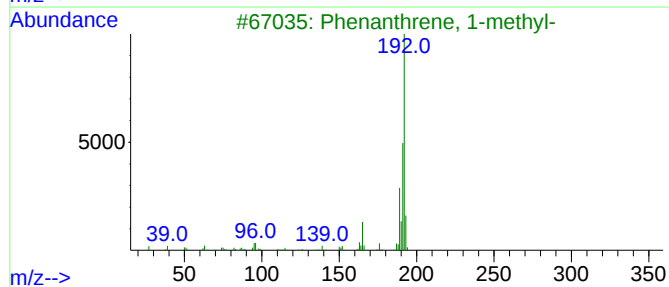
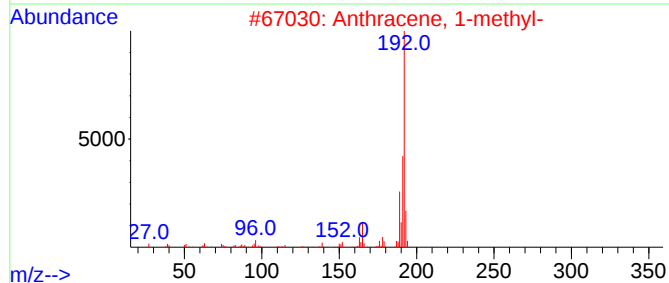
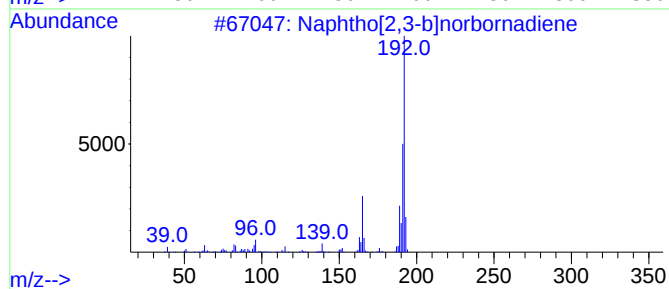
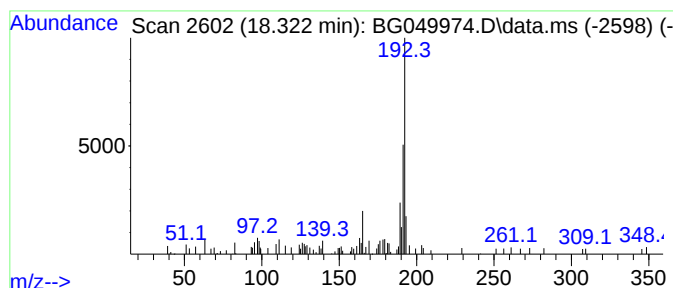
Instrument :
BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Naphtho[2,3-b]norbornadiene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.322	2.27 ng	45683	Phenanthrene-d10		17.394	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Naphtho[2,3-b]norbornadiene		192	C15H12	107426-38-0	93
2	Anthracene, 1-methyl-		192	C15H12	000610-48-0	91
3	Phenanthrene, 1-methyl-		192	C15H12	000832-69-9	87
4	Phenanthrene, 2-methyl-		192	C15H12	002531-84-2	87
5	1H-Indene, 2-phenyl-		192	C15H12	004505-48-0	87



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Instrument :
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ClientSampleId :
PL-01-082421

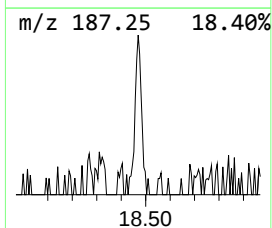
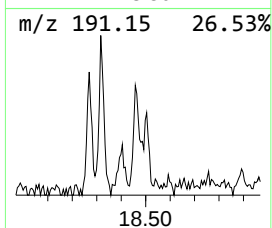
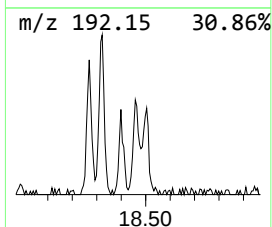
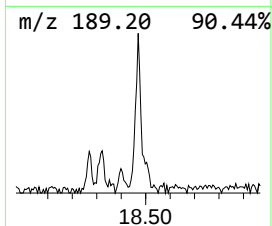
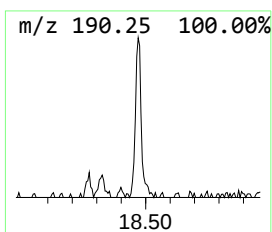
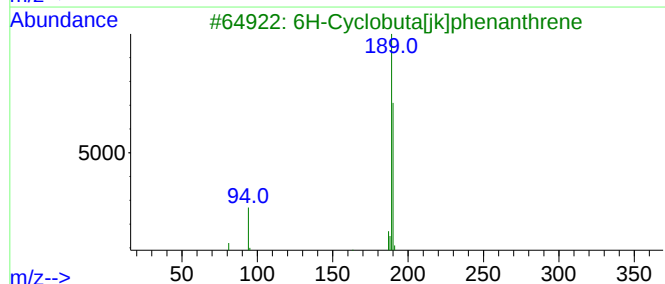
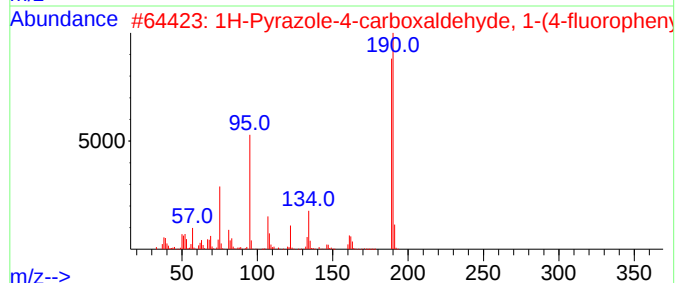
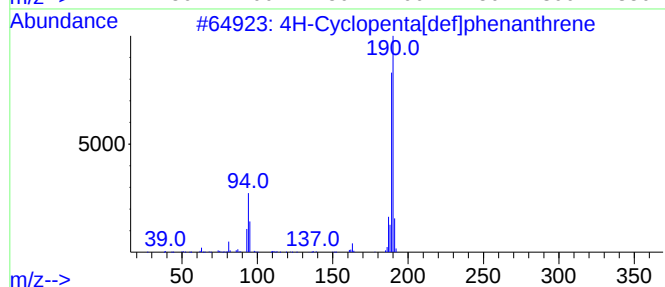
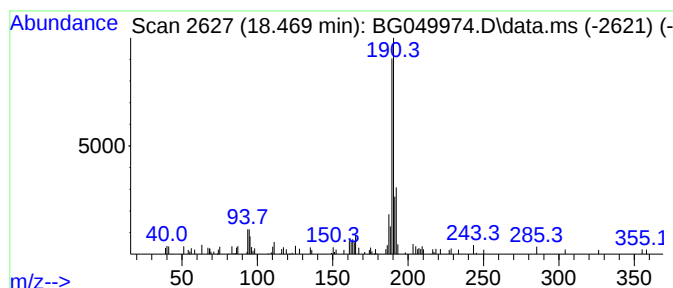
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.469	3.74 ng	75341	Phenanthrene-d10	17.394

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	72
2			1H-Pyrazole-4-carboxaldehyde, 1-(4-fluorophenyl)	190	C10H7FN2O	1000338-05-6	52
3			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	50
4			1,4-Naphthalenedione, 2,5-dihydro	190	C10H6O4	004923-55-1	35
5			Benzimidazol-2(3H)-one, 5-formyl	190	C10H10N2O2	055241-49-1	33



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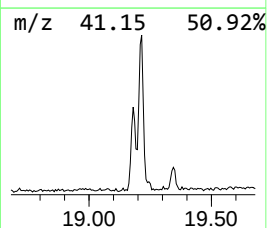
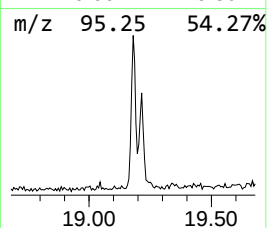
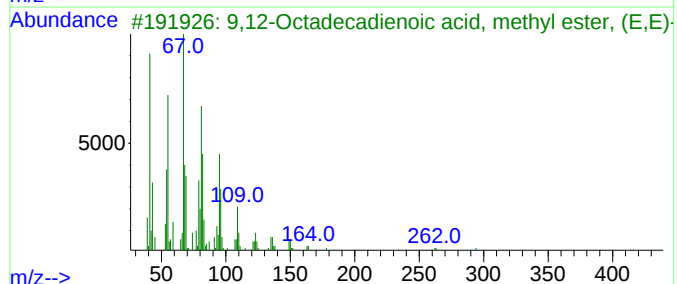
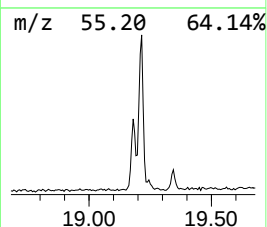
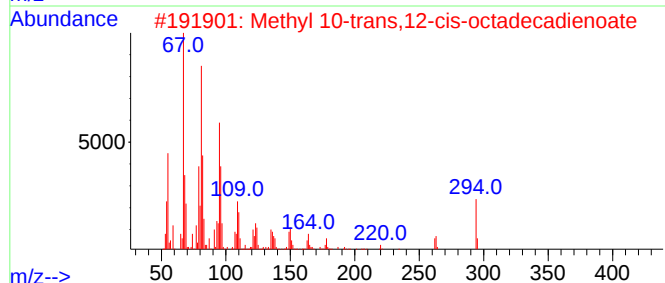
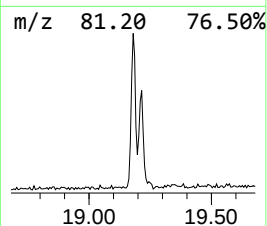
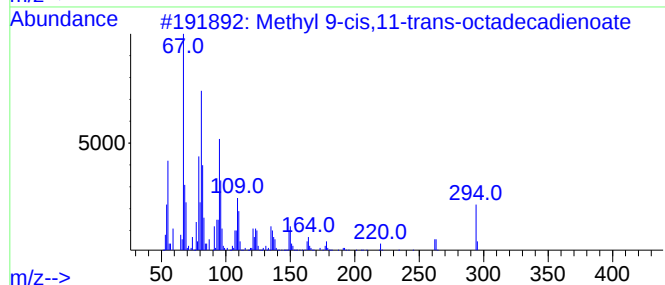
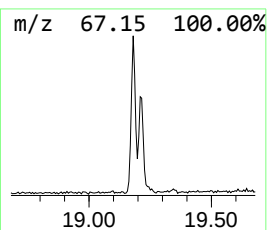
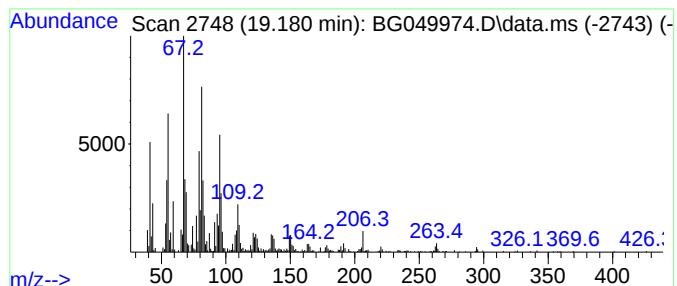
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Methyl 9-cis,11-trans-octad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.180	28.24 ng	568444	Phenanthrene-d10	17.394

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	99
2			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	96
4			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96
5			11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049974.D
Acq On : 25 Aug 2021 18:59
Operator : CG/JU
Sample : M3530-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PL-01-082421

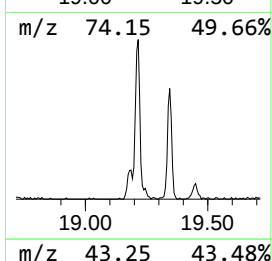
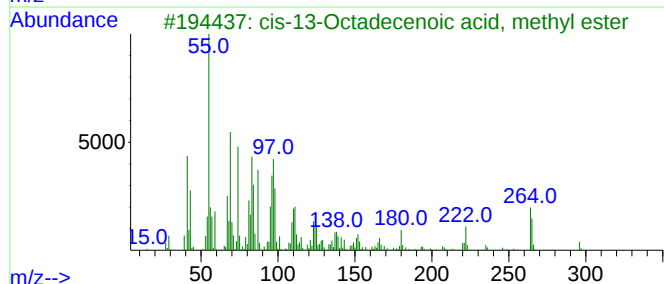
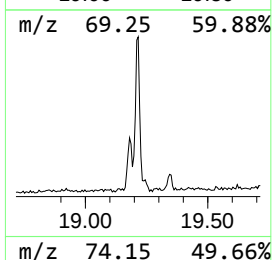
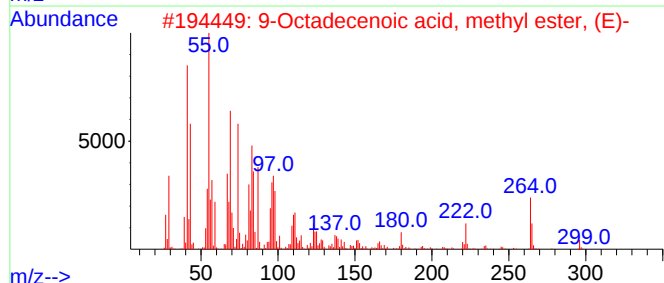
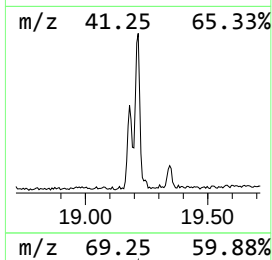
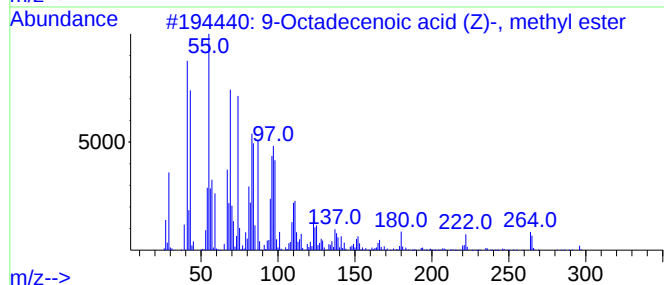
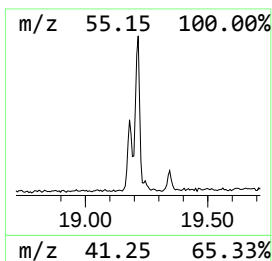
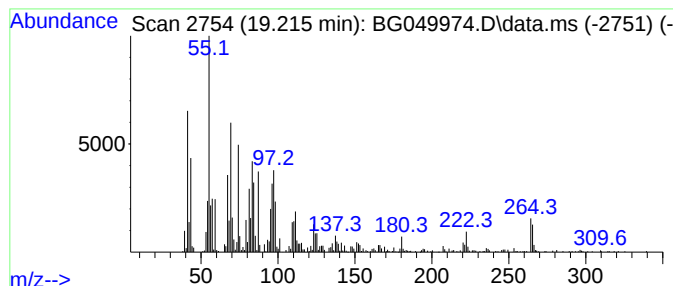
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.215	34.64 ng	697287	Phenanthrene-d10	17.394

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
3			cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	94
4			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	94
5			8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049974.D
Acq On : 25 Aug 2021 18:59
Operator : CG/JU
Sample : M3530-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

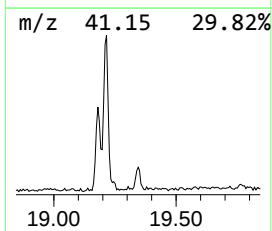
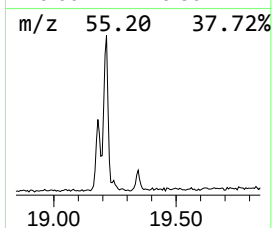
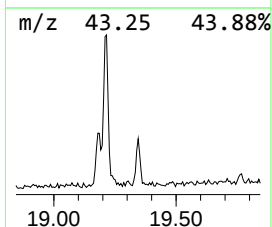
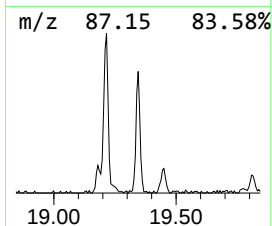
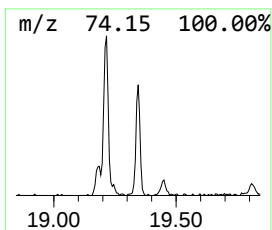
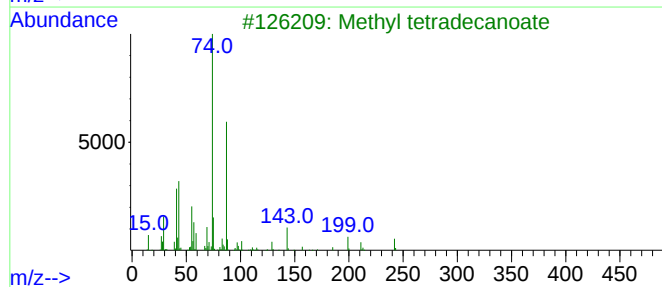
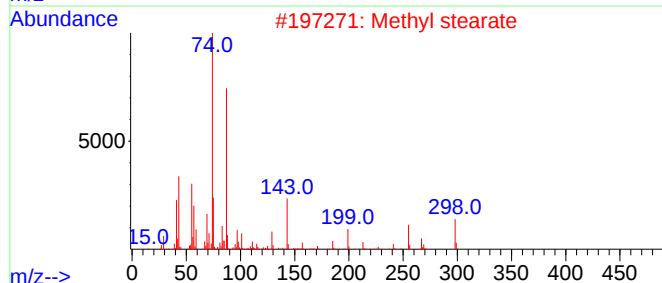
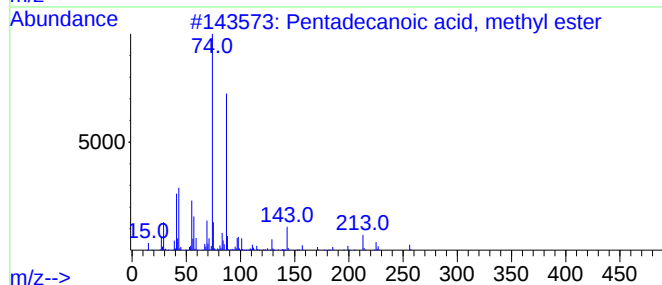
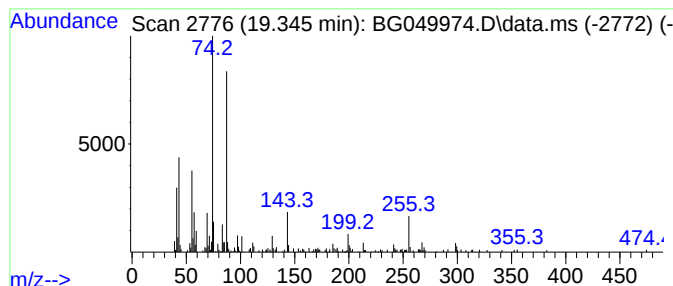
Instrument :
BNA_G
ClientSampleId :
PL-01-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentadecanoic acid, methyl ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.345	6.67 ng	134343	Phenanthrene-d10		17.394	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	91
2	Methyl stearate		298	C19H38O2	000112-61-8	87
3	Methyl tetradecanoate		242	C15H30O2	000124-10-7	87
4	Heptadecanoic acid, 16-methyl-, ...		298	C19H38O2	005129-61-3	86
5	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082521\
Data File : BG049974.D
Acq On : 25 Aug 2021 18:59
Operator : CG/JU
Sample : M3530-01 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PL-01-082421

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Hexadecanoic ac...	18.040	11.4	ng	229308	4	17.394	402596	20.0
Naphtho[2,3-b]n...	18.322	2.3	ng	45683	4	17.394	402596	20.0
4H-Cyclopenta[d...	18.469	3.7	ng	75341	4	17.394	402596	20.0
Methyl 9-cis,11...	19.180	28.2	ng	568444	4	17.394	402596	20.0
9-Octadecenoic ...	19.215	34.6	ng	697287	4	17.394	402596	20.0
Pentadecanoic a...	19.345	6.7	ng	134343	4	17.394	402596	20.0