

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
 Data File : BG048036.D
 Acq On : 27 Jan 2021 20:16
 Operator : CG/JU
 Sample : M1226-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0049-043-COMP-C-ELUTRIATE

Integration Parameters: rteint.p

Integrator: RTE

Smoother: 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-BG012521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.677	390	398	406	rBV	448809	714876	25.36%	3.841%
2	7.269	661	669	680	rBV2	328190	651736	23.12%	3.502%
3	8.121	808	814	821	rBV	179706	302041	10.71%	1.623%
4	9.285	1003	1012	1021	rVB	432534	773260	27.43%	4.155%
5	10.936	1285	1293	1301	rBV	228821	410719	14.57%	2.207%
6	13.374	1700	1708	1717	rVB	1146957	1717873	60.93%	9.230%
7	13.574	1732	1742	1749	rBV3	29742	55167	1.96%	0.296%
8	14.191	1841	1847	1851	rBV	67548	94383	3.35%	0.507%
9	14.379	1875	1879	1886	rBV5	26340	43081	1.53%	0.231%
10	14.743	1935	1941	1950	rVB2	369320	599526	21.27%	3.221%
11	15.142	2004	2009	2014	rBV4	22768	37195	1.32%	0.200%
12	15.542	2072	2077	2082	rBV3	21693	40340	1.43%	0.217%
13	16.229	2186	2194	2200	rBV	999897	1516636	53.80%	8.149%
14	16.623	2255	2261	2267	rBV9	14730	30516	1.08%	0.164%
15	16.723	2274	2278	2284	rBV2	27578	35249	1.25%	0.189%
16	17.399	2388	2393	2397	rVB3	26208	33830	1.20%	0.182%
17	17.487	2402	2408	2415	rVV	531427	772213	27.39%	4.149%
18	17.763	2451	2455	2458	rBV	30544	43658	1.55%	0.235%
19	18.374	2553	2559	2567	rBV	850582	1151824	40.86%	6.189%
20	18.444	2567	2571	2576	rVB	50622	77312	2.74%	0.415%
21	18.879	2641	2645	2650	rBV2	38468	62856	2.23%	0.338%
22	19.138	2684	2689	2694	rBV	307869	377602	13.39%	2.029%
23	19.226	2699	2704	2708	rBV	97338	118240	4.19%	0.635%
24	19.290	2711	2715	2721	rVB2	34864	49790	1.77%	0.268%
25	19.490	2745	2749	2751	rBV2	31961	40176	1.43%	0.216%
26	19.637	2769	2774	2784	rBV	676447	862821	30.61%	4.636%
27	19.766	2792	2796	2803	rVB	105325	132798	4.71%	0.714%
28	19.831	2804	2807	2810	rBV2	30525	37822	1.34%	0.203%
29	19.896	2815	2818	2822	rVB6	22527	31037	1.10%	0.167%
30	20.089	2845	2851	2856	rBV2	2126627	2819212	100.00%	15.147%
31	20.295	2882	2886	2891	rVB	72468	96559	3.43%	0.519%
32	20.360	2891	2897	2900	rBV5	41842	75674	2.68%	0.407%
33	20.507	2920	2922	2926	rVB2	28329	29418	1.04%	0.158%
34	20.771	2964	2967	2973	rVB	139324	178780	6.34%	0.961%
35	20.994	3000	3005	3009	rBV	574930	729862	25.89%	3.922%
36	21.041	3009	3013	3017	rVV	143347	177928	6.31%	0.956%

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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

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37	21.106	3021	3024	3034	rVB2	52014	77624	2.75%	0.417%
38	21.400	3069	3074	3083	rBV	499820	768481	27.26%	4.129%
39	21.476	3084	3087	3094	rVB	33460	43430	1.54%	0.233%
40	21.552	3096	3100	3107	rVB2	63292	95908	3.40%	0.515%
41	21.629	3110	3113	3116	rBV3	23008	31564	1.12%	0.170%
42	21.764	3129	3136	3142	rVB	574879	966390	34.28%	5.192%
43	21.964	3166	3170	3175	rVB3	36622	50877	1.80%	0.273%
44	22.592	3273	3277	3286	rVB5	40533	103652	3.68%	0.557%
45	23.297	3393	3397	3403	rVB4	37775	56598	2.01%	0.304%
46	23.497	3426	3431	3438	rVB2	34012	62813	2.23%	0.337%
47	24.126	3534	3538	3544	rVB4	42995	80568	2.86%	0.433%
48	25.043	3685	3694	3715	rVB2	335018	1053132	37.36%	5.658%
49	26.270	3897	3903	3911	rVB8	26072	70087	2.49%	0.377%
50	26.394	3917	3924	3935	rVB6	74071	228634	8.11%	1.228%

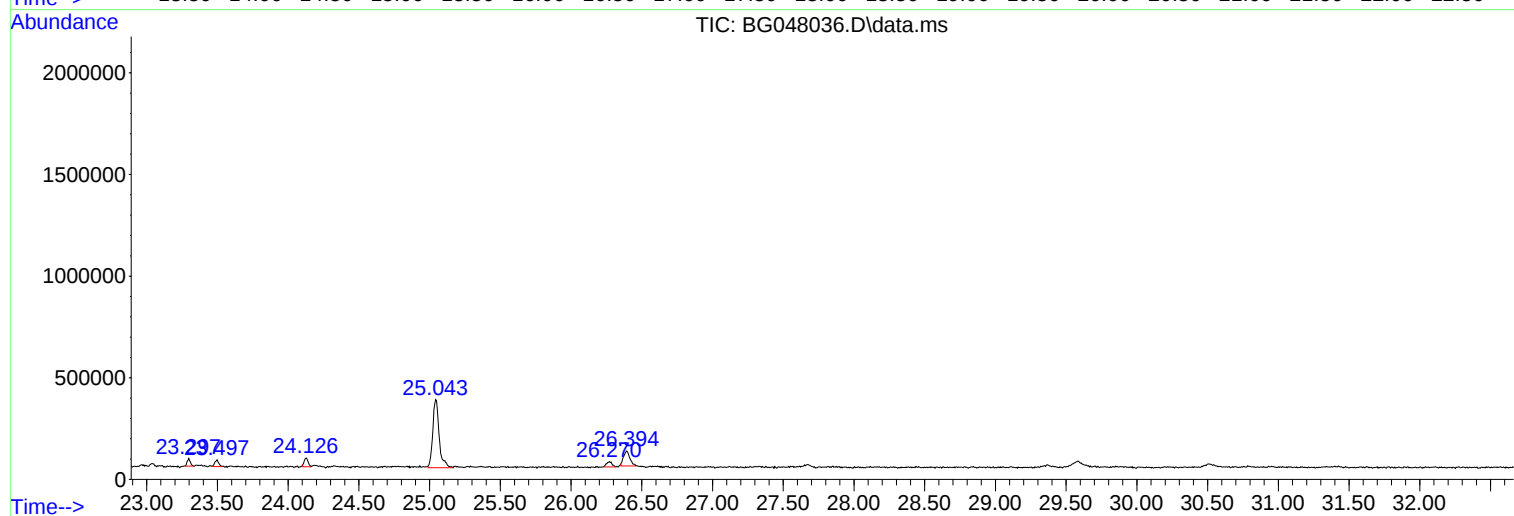
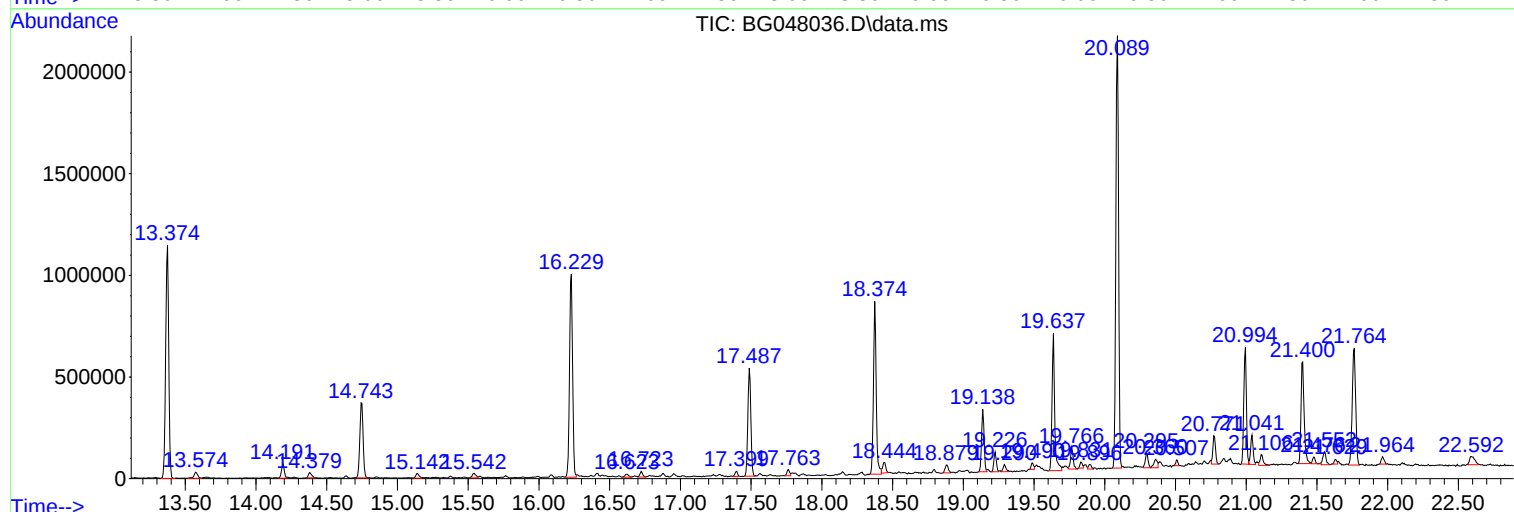
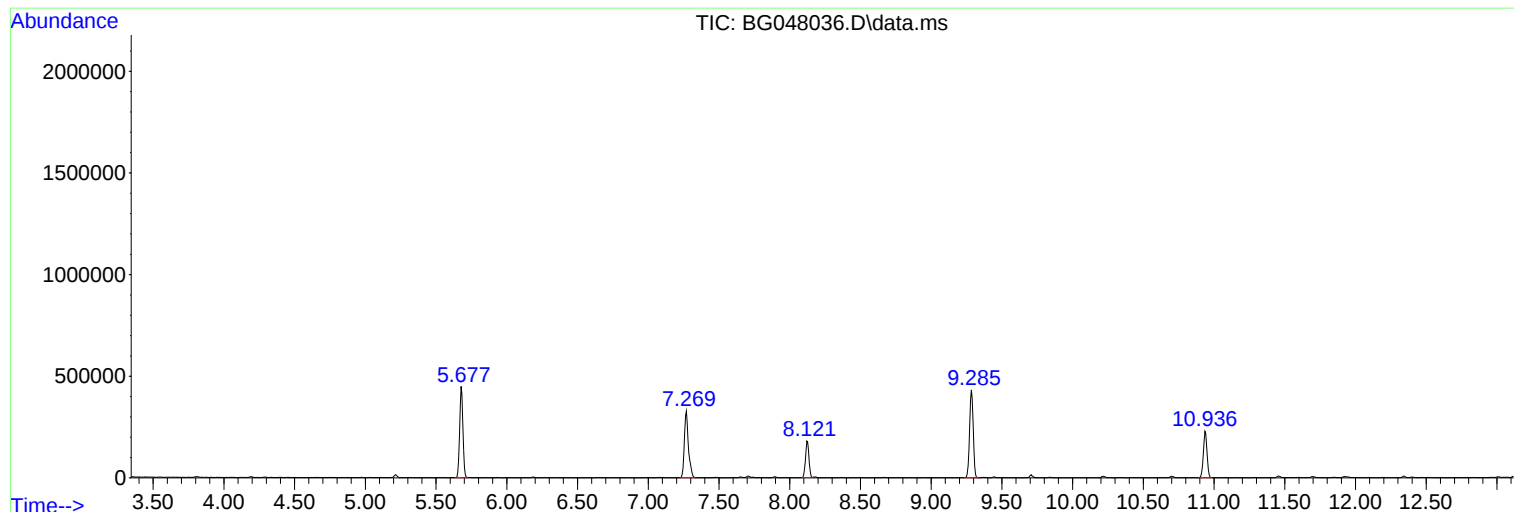
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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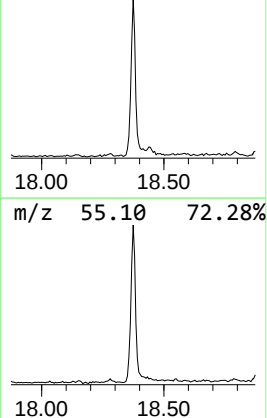
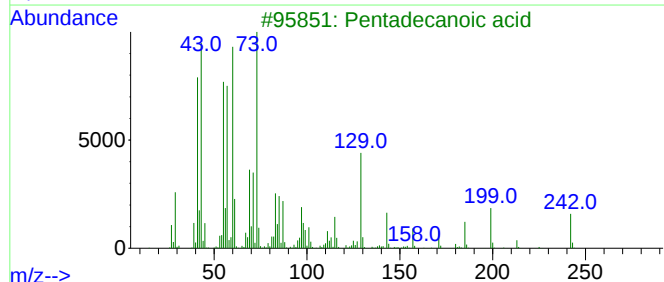
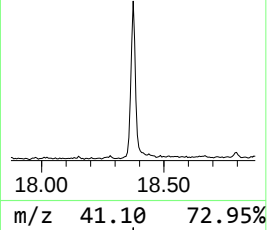
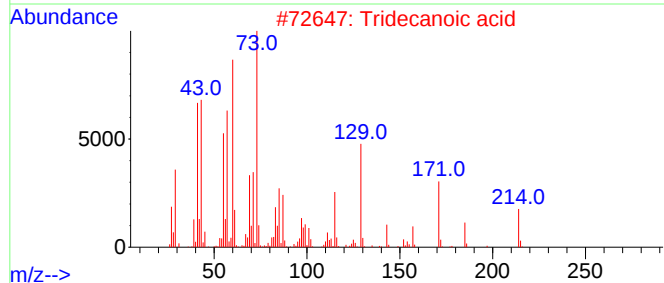
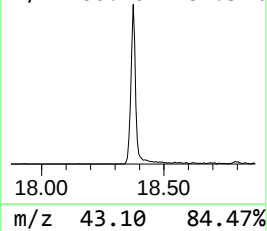
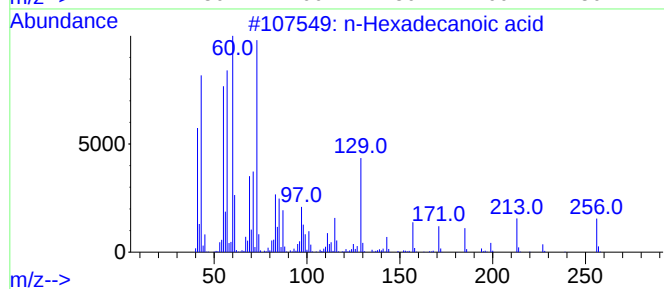
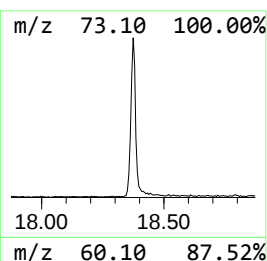
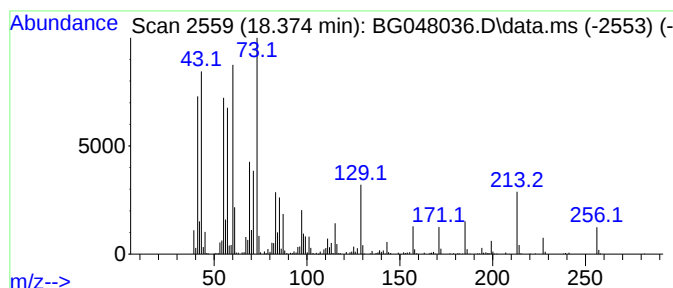
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	29.83 ng	1151820	Phenanthrene-d10	17.487

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	20



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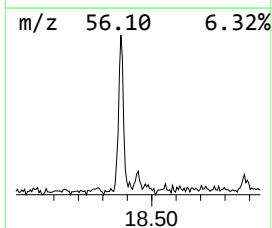
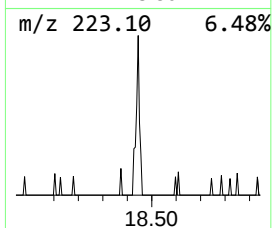
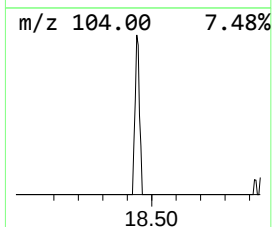
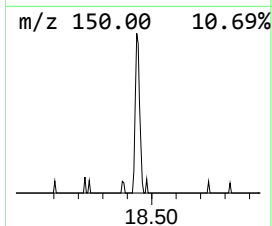
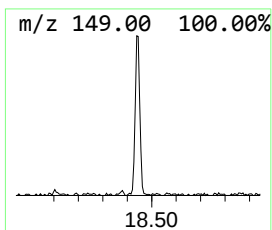
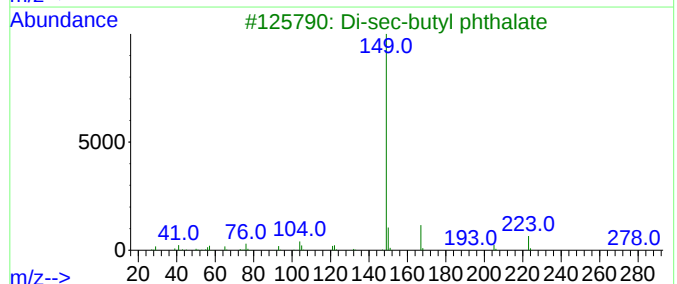
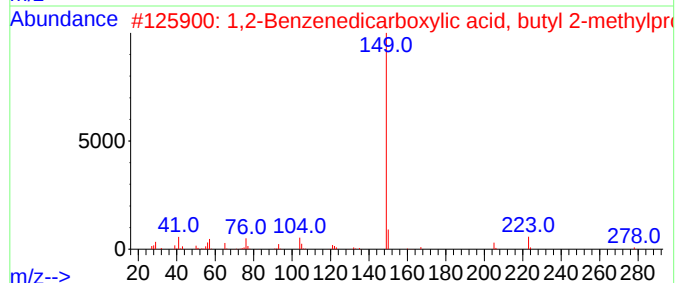
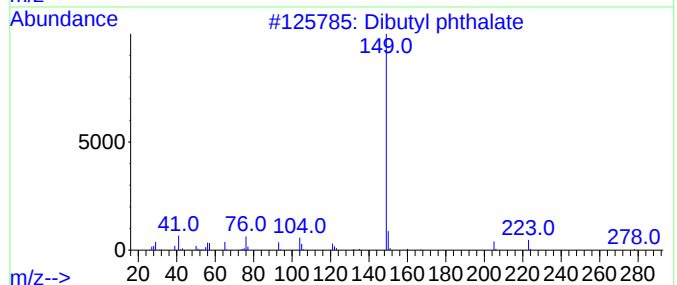
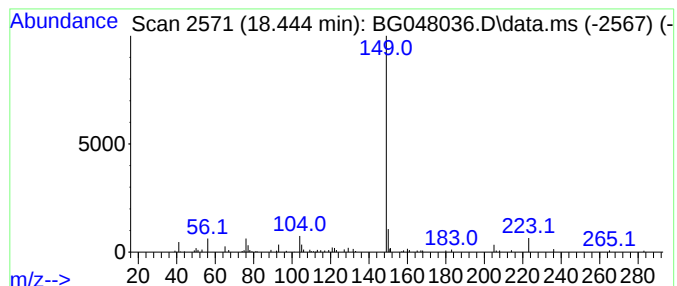
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.444	2.00 ng	77312	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibutyl phthalate	278	C16H22O4	000084-74-2	80
2			1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	80
3			Di-sec-butyl phthalate	278	C16H22O4	1000373-65-4	78
4			1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	72
5			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	72



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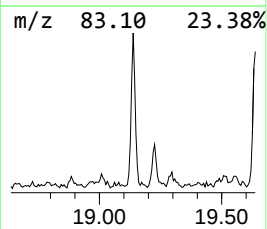
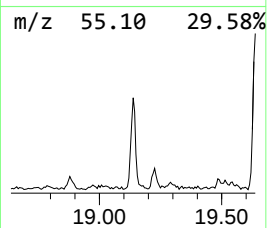
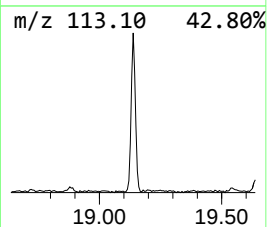
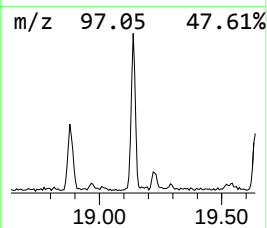
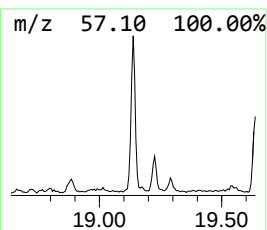
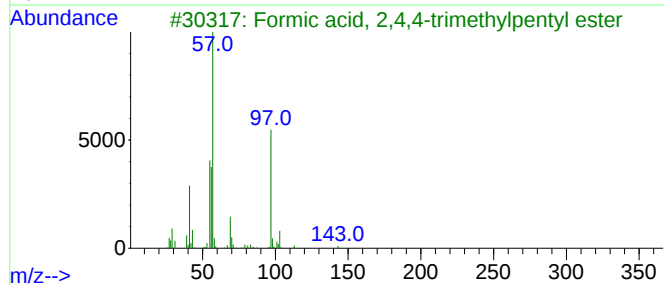
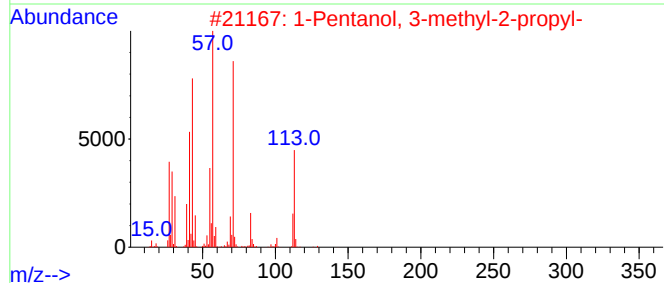
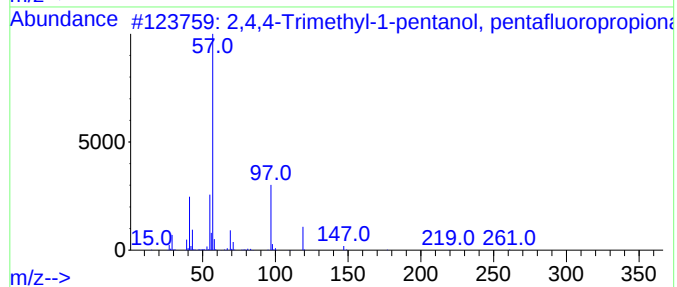
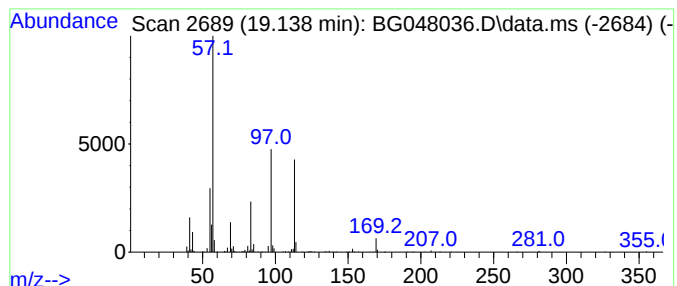
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown19.138 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.138	9.78 ng	377602	Phenanthrene-d10	17.487

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32
2		1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
3		Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25
4		Octane, 2-bromo-	192	C8H17Br	000557-35-7	25
5		4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	25



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Instrument :
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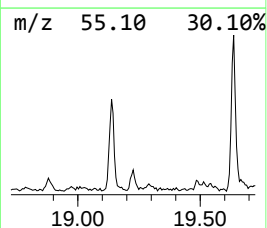
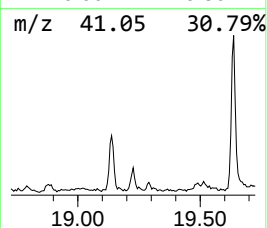
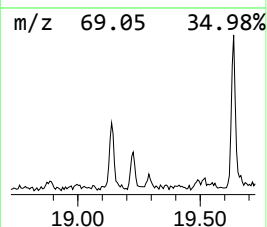
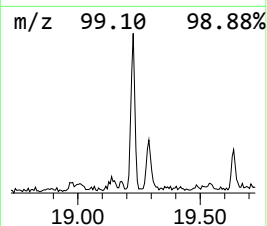
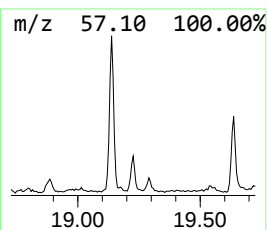
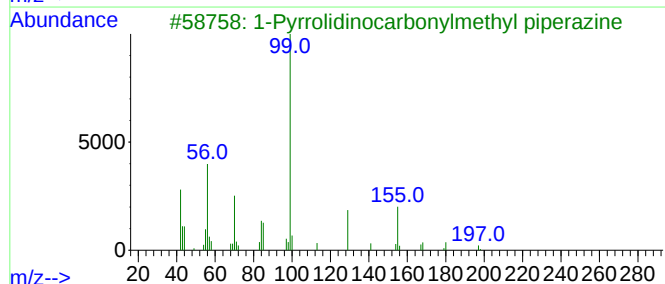
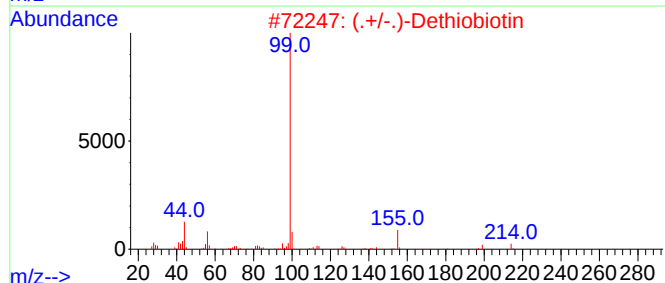
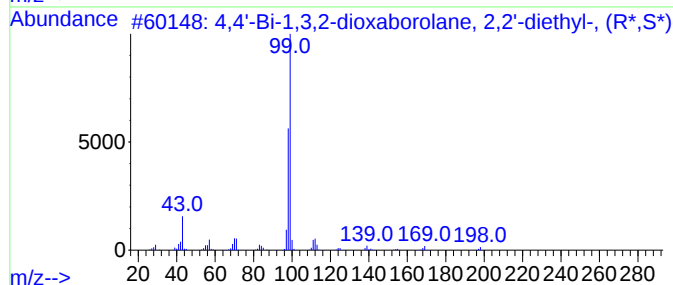
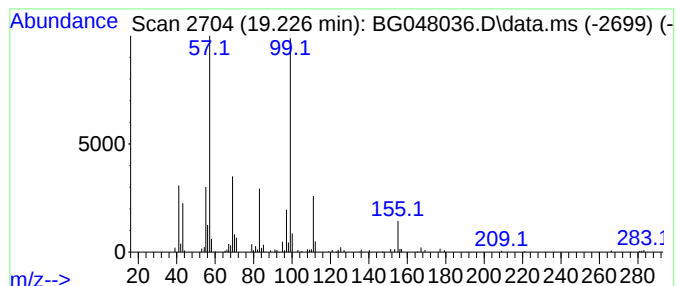
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown19.226 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.226	3.06 ng	118240	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bi-1,3,2-dioxaborolane, 2,2...	198	C8H16B2O4	062337-94-4	43		
2	(.+/-)-Dethiobiotin	214	C10H18N2O3	000636-20-4	43		
3	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	43		
4	Phosphoric acid, monododecyl ester	266	C12H27O4P	002627-35-2	38		
5	Hexanoic acid, 5-tridecyl ester	298	C19H38O2	1000279-29-4	38		



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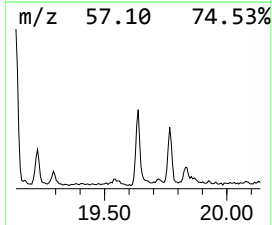
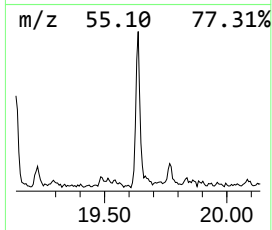
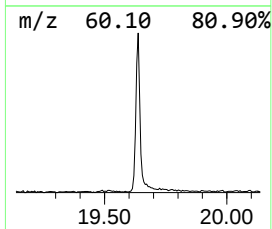
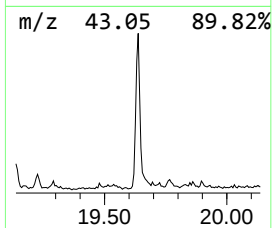
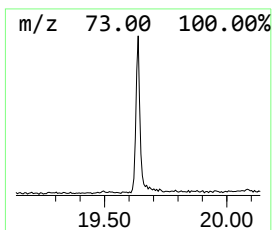
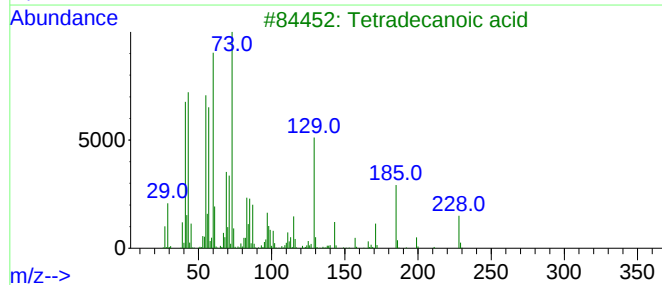
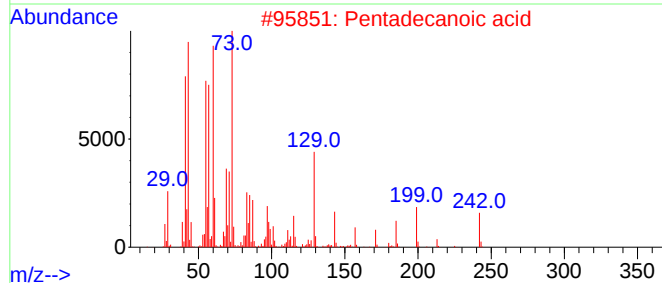
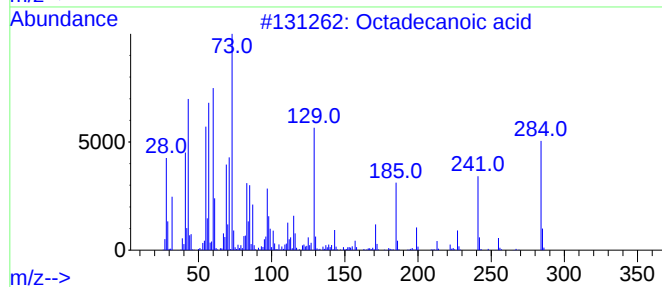
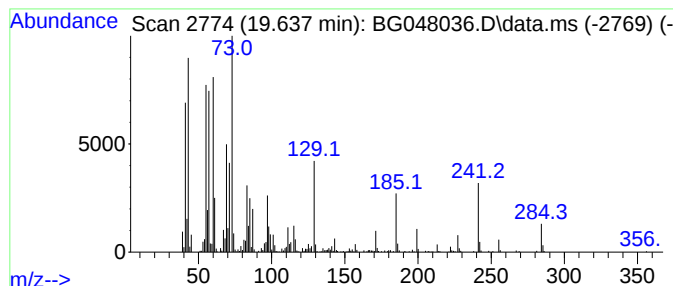
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.637	17.86 ng	862821	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

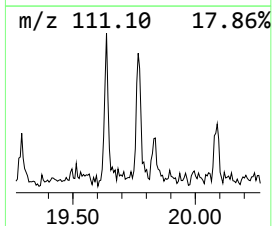
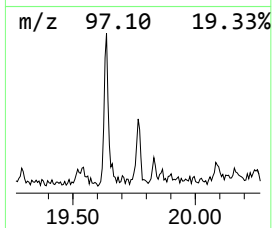
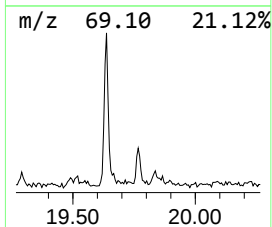
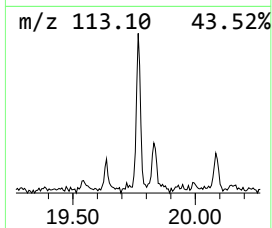
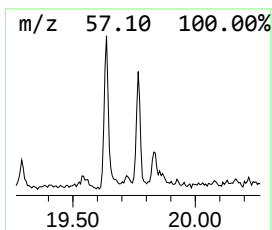
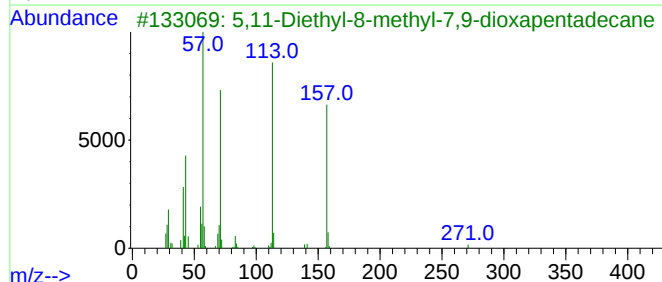
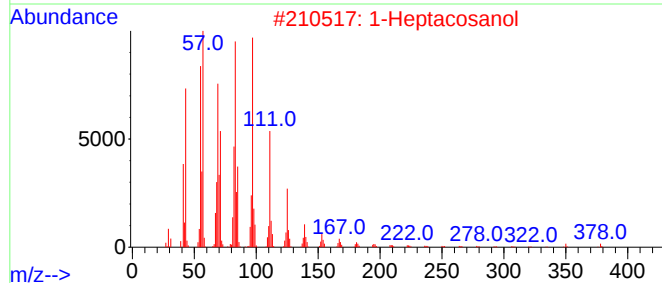
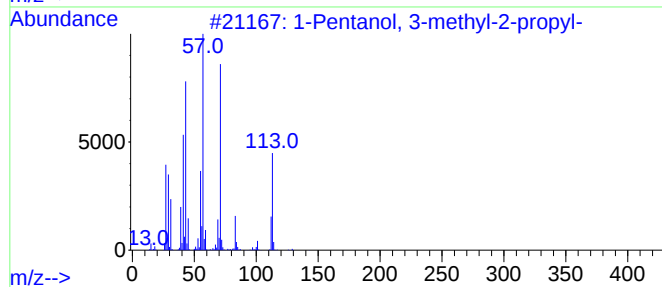
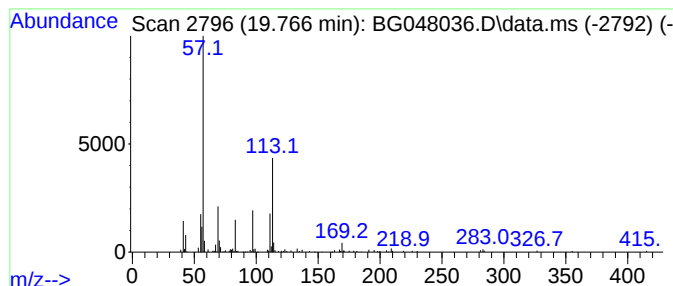
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown19.766 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.766	2.75 ng	132798	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	33		
2	1-Heptacosanol	396	C27H56O	002004-39-9	25		
3	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	23		
4	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	17		
5	Tetratriacontyl heptafluorobutyrate	691	C38H69F7O2	1000351-84-1	17		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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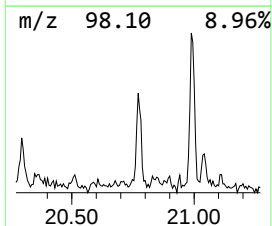
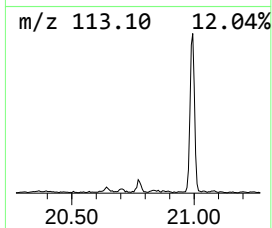
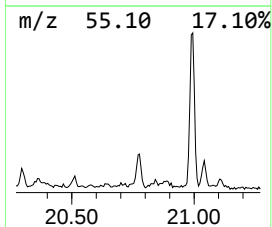
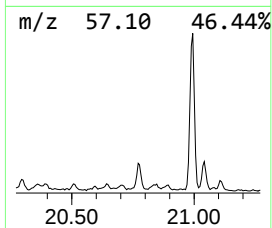
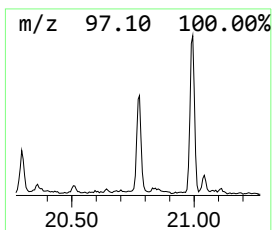
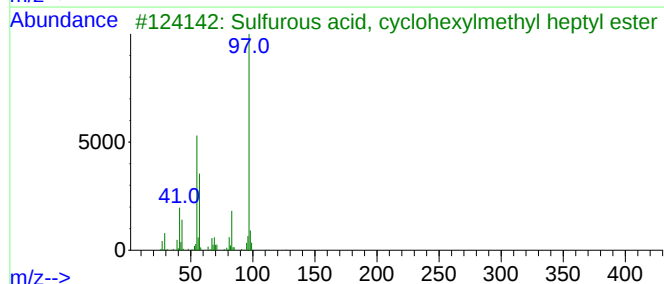
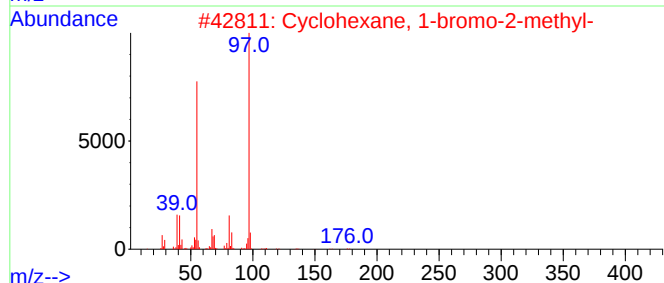
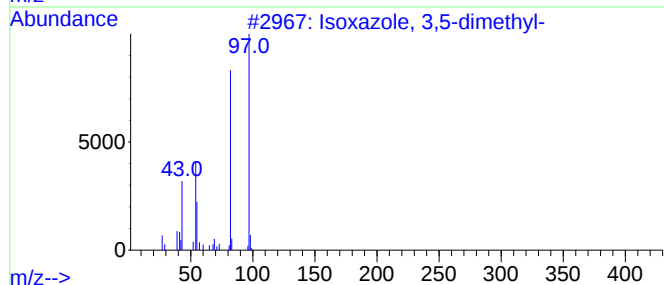
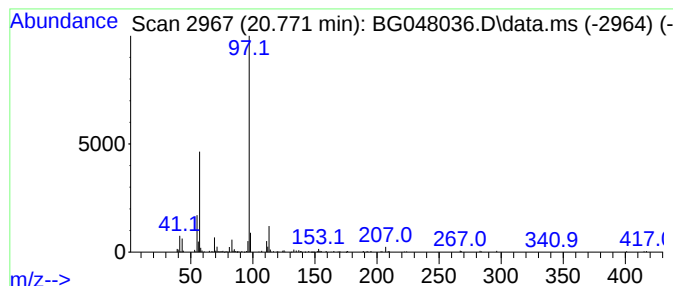
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Isoxazole, 3,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.771	3.70 ng	178780	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isoxazole, 3,5-dimethyl-	97	C5H7NO	000300-87-8	53
2			Cyclohexane, 1-bromo-2-methyl-	176	C7H13Br	006294-39-9	53
3			Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	45
4			Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	42
5			Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	006294-40-2	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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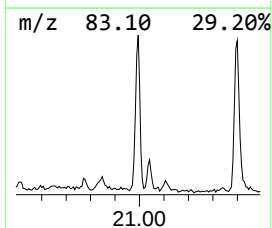
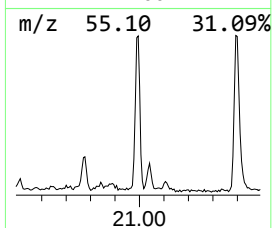
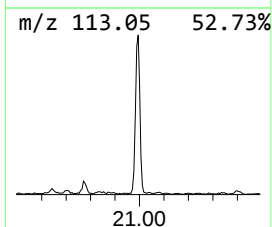
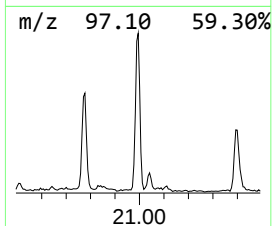
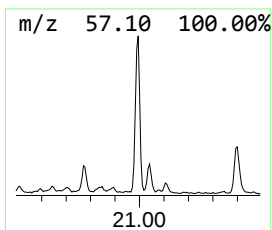
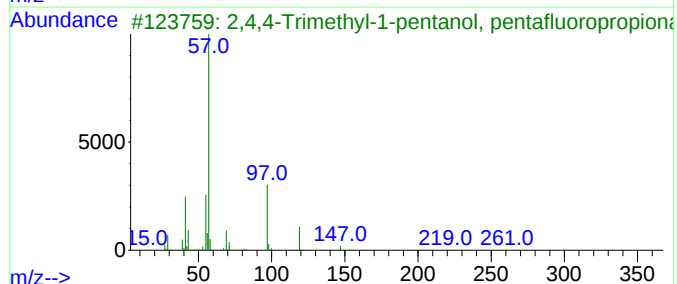
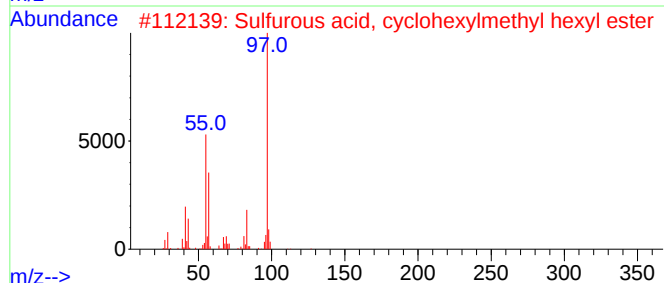
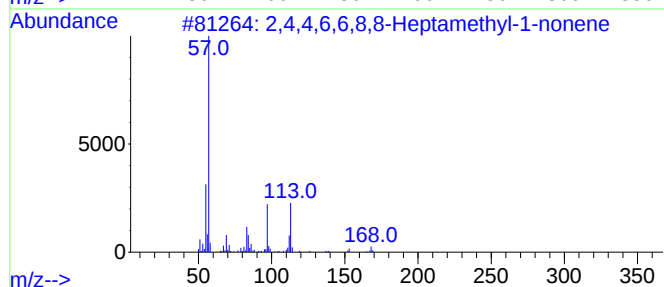
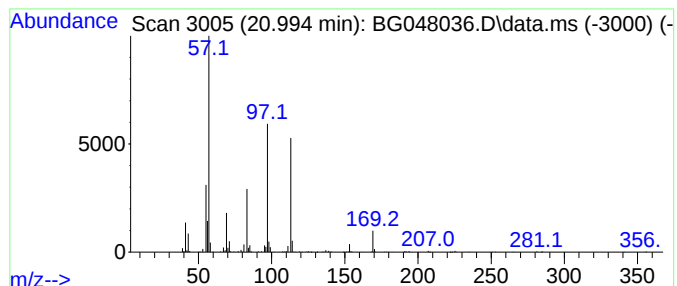
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown20.994 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.994	15.10 ng	729862	Chrysene-d12	21.764

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	40		
2	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	38		
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	35		
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32		
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	27		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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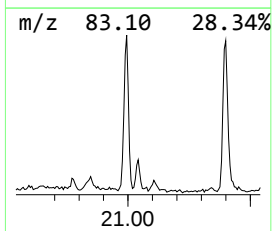
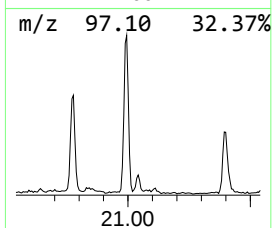
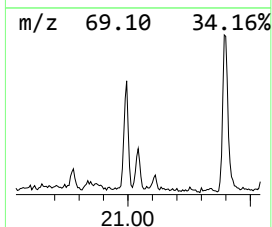
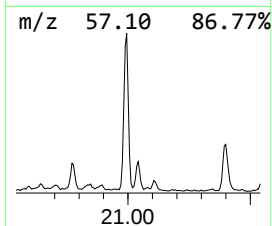
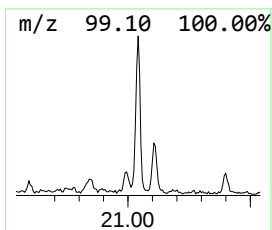
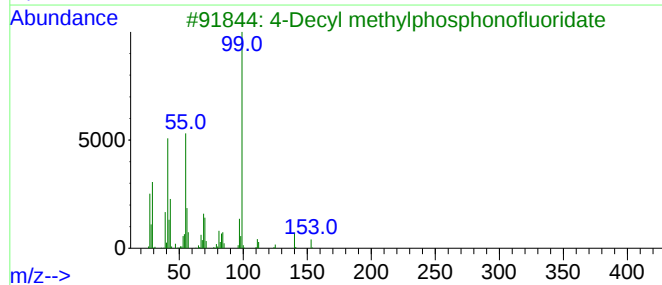
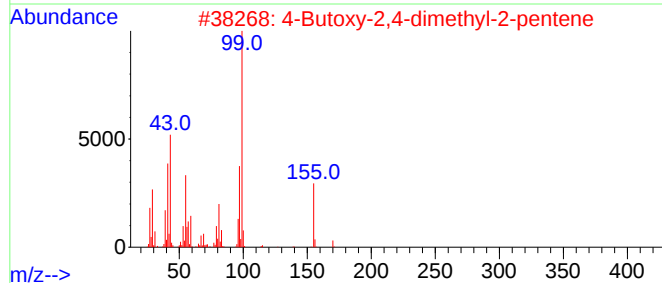
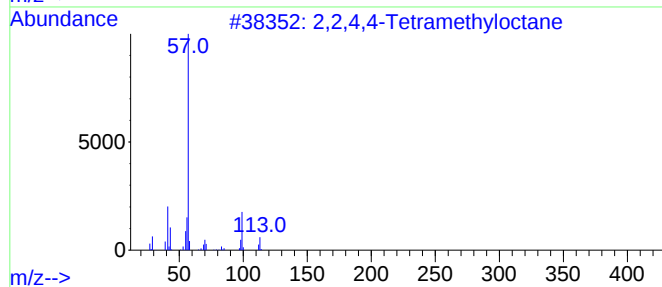
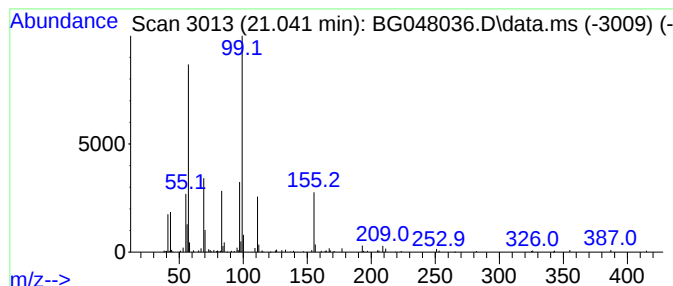
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown21.041 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.041	3.68 ng	177928	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4,4-Tetramethyloctane	170	C12H26	062183-79-3	43		
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	42		
3	4-Decyl methylphosphonofluoridate	238	C11H24F02P	1000216-71-5	38		
4	2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	37		
5	Hexanamide, N-hexanoyl-N-allyl-	253	C15H27NO2	1000340-15-1	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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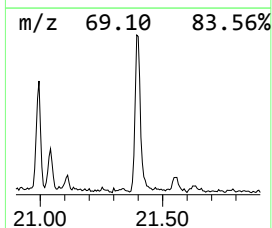
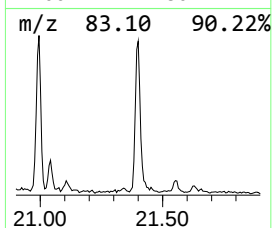
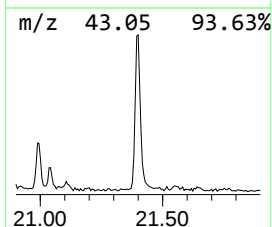
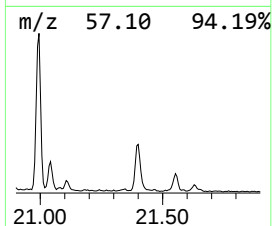
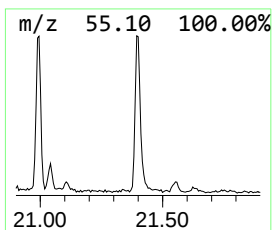
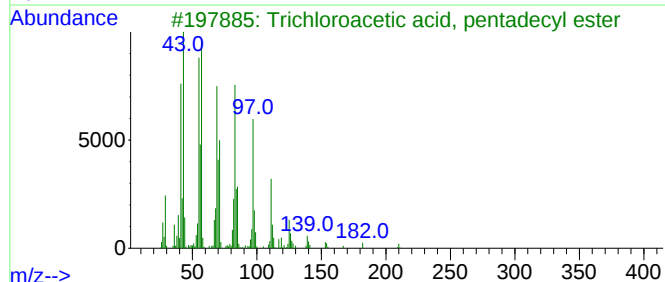
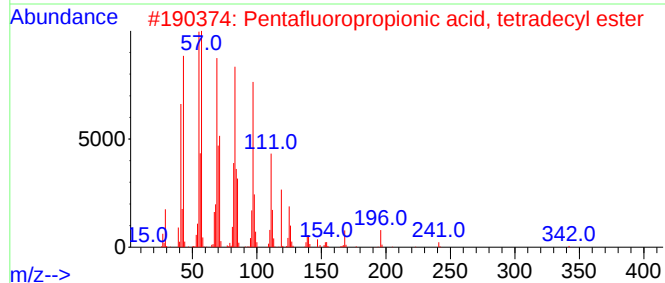
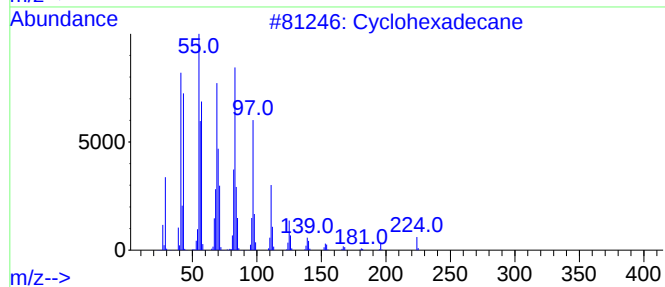
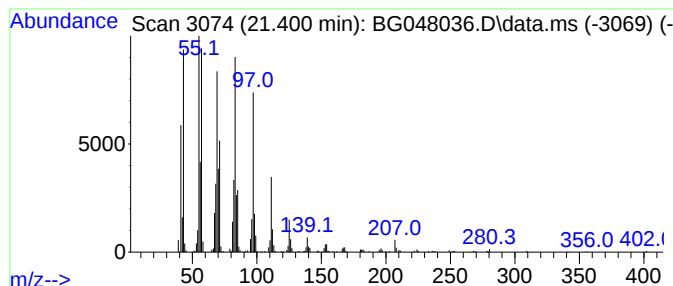
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.400	15.90 ng	768481	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	98
2			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
3			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
0049-043-COMP-C-ELUTRIATE

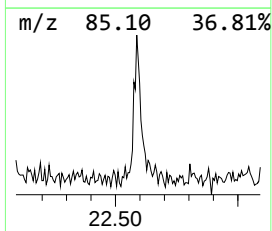
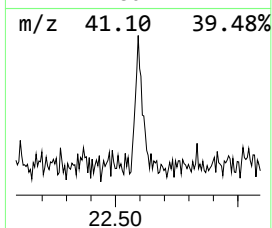
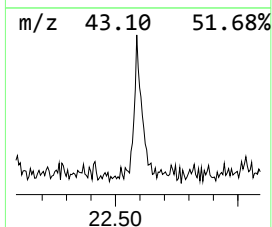
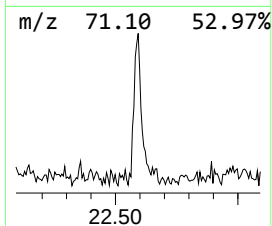
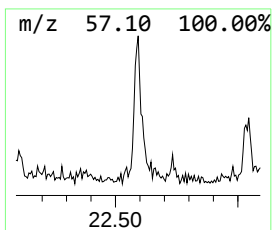
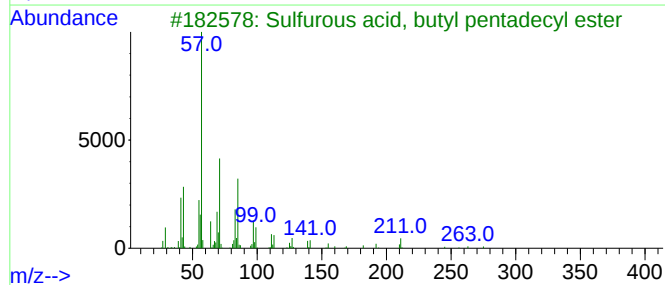
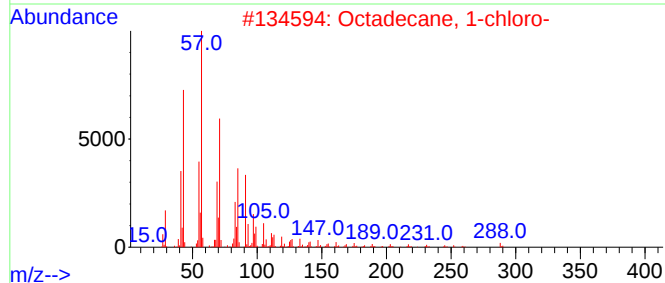
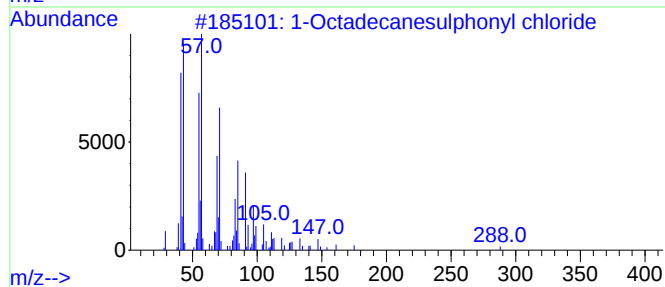
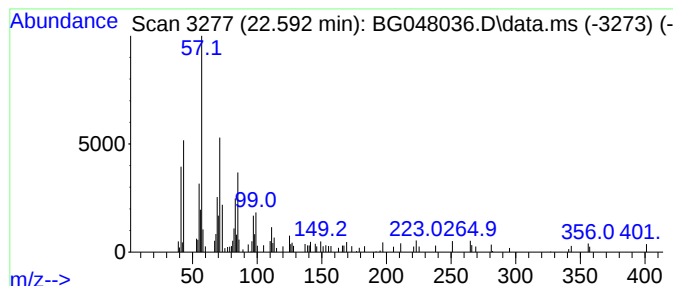
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Octadecanesulphonyl chloride Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.592	2.15 ng	103652	Chrysene-d12	21.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	53
2			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	49
3			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	49
4			Tritetracontane	605	C43H88	007098-21-7	49
5			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048036.D
Acq On : 27 Jan 2021 20:16
Operator : CG/JU
Sample : M1226-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

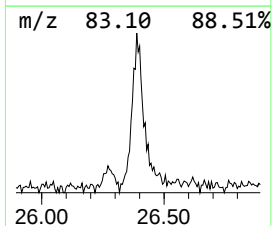
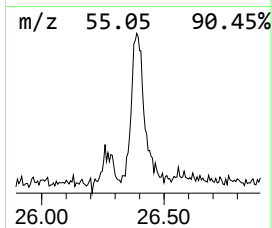
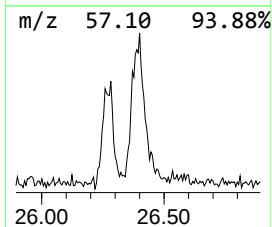
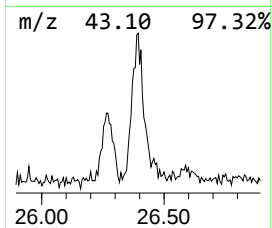
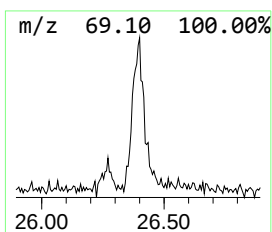
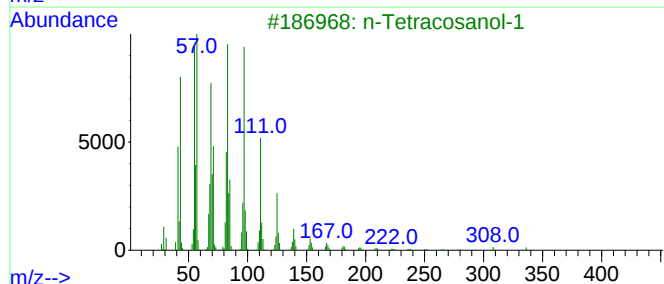
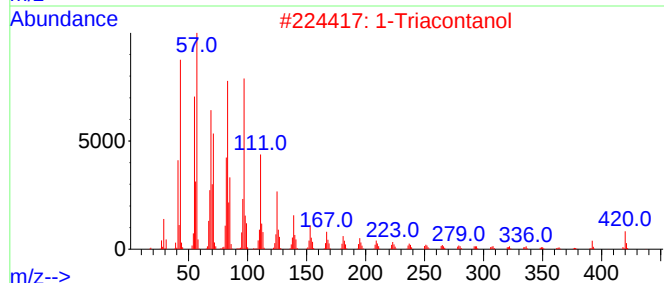
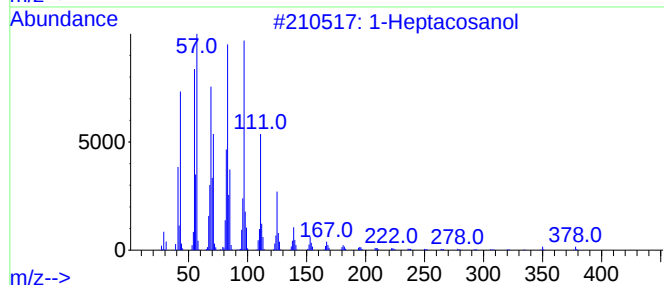
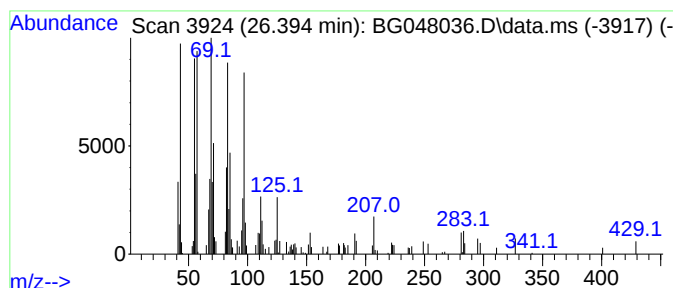
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.394	4.34 ng	228634	Perylene-d12	25.043

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol		396	C27H56O	002004-39-9	81
2	1-Triacontanol		438	C30H62O	000593-50-0	58
3	n-Tetracosanol-1		354	C24H50O	000506-51-4	58
4	1-Hexacosanol		382	C26H54O	000506-52-5	58
5	Fumaric acid, 2-chloropropyl tri...		374	C20H35ClO4	1000348-57-1	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
 Data File : BG048036.D
 Acq On : 27 Jan 2021 20:16
 Operator : CG/JU
 Sample : M1226-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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
n-Hexadecanoic ...	18.374	29.8	ng	1151820	4	17.487	772213	20.0
1,2-Benzenedica...	18.444	2.0	ng	77312	4	17.487	772213	20.0
unknown19.138	19.138	9.8	ng	377602	4	17.487	772213	20.0
unknown19.226	19.226	3.1	ng	118240	4	17.487	772213	20.0
Octadecanoic acid	19.637	17.9	ng	862821	5	21.764	966390	20.0
unknown19.766	19.766	2.8	ng	132798	5	21.764	966390	20.0
Isoxazole, 3,5-...	20.771	3.7	ng	178780	5	21.764	966390	20.0
unknown20.994	20.994	15.1	ng	729862	5	21.764	966390	20.0
unknown21.041	21.041	3.7	ng	177928	5	21.764	966390	20.0
Cyclohexadecane	21.400	15.9	ng	768481	5	21.764	966390	20.0
1-Octadecanesul...	22.592	2.1	ng	103652	5	21.764	966390	20.0
1-Heptacosanol	26.394	4.3	ng	228634	6	25.043	1053130	20.0