

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110522\
 Data File : BG055473.D
 Acq On : 5 Nov 2022 16:48
 Operator : CG/JU
 Sample : N5418-16
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-O

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-BG110122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055473.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.274	332	338	347	rBV	85886	136736	8.31%	1.525%
2	5.756	414	420	436	rBV	357803	599555	36.44%	6.688%
3	7.383	689	697	709	rBV	358956	638215	38.79%	7.119%
4	8.229	834	841	847	rBV	96776	165241	10.04%	1.843%
5	9.404	1031	1041	1054	rBV	226926	401674	24.42%	4.481%
6	11.055	1315	1322	1330	rBV	141542	243219	14.78%	2.713%
7	13.470	1725	1733	1741	rBV	703942	1032702	62.77%	11.520%
8	14.845	1960	1967	1974	rBV	237453	345667	21.01%	3.856%
9	16.326	2213	2219	2234	rBV	545994	848847	51.60%	9.469%
10	17.577	2424	2432	2437	rBV	282914	432493	26.29%	4.824%
11	17.618	2437	2439	2445	rVB	28303	36980	2.25%	0.413%
12	18.447	2572	2580	2585	rBV4	19613	45153	2.74%	0.504%
13	18.500	2585	2589	2595	rVB2	17466	27748	1.69%	0.310%
14	18.641	2607	2613	2616	rBV4	10864	19848	1.21%	0.221%
15	19.346	2727	2733	2738	rBV3	12514	22256	1.35%	0.248%
16	19.610	2773	2778	2784	rBV	62115	89534	5.44%	0.999%
17	19.692	2785	2792	2801	rBV6	27327	79492	4.83%	0.887%
18	19.974	2835	2840	2847	rVB	71392	107307	6.52%	1.197%
19	20.151	2864	2870	2876	rBV	1243323	1645156	100.00%	18.352%
20	20.427	2912	2917	2919	rBV6	15716	24060	1.46%	0.268%
21	21.455	3087	3092	3107	rVB7	49921	157407	9.57%	1.756%
22	21.849	3150	3159	3164	rBV	324604	629643	38.27%	7.024%
23	21.896	3164	3167	3175	rVB	45506	76017	4.62%	0.848%
24	22.618	3286	3290	3294	rVB3	17228	27190	1.65%	0.303%
25	22.689	3296	3302	3312	rVV9	20981	68591	4.17%	0.765%
26	23.329	3405	3411	3419	rVB3	34057	68209	4.15%	0.761%
27	23.535	3442	3446	3454	rVB	16381	30439	1.85%	0.340%
28	23.705	3469	3475	3482	rVB3	42787	89159	5.42%	0.995%
29	24.164	3544	3553	3566	rBV2	51614	178144	10.83%	1.987%
30	24.904	3673	3679	3685	rVB2	14651	35115	2.13%	0.392%
31	25.221	3723	3733	3743	rVB2	186408	533797	32.45%	5.954%
32	26.320	3914	3920	3932	rVB3	42137	129082	7.85%	1.440%

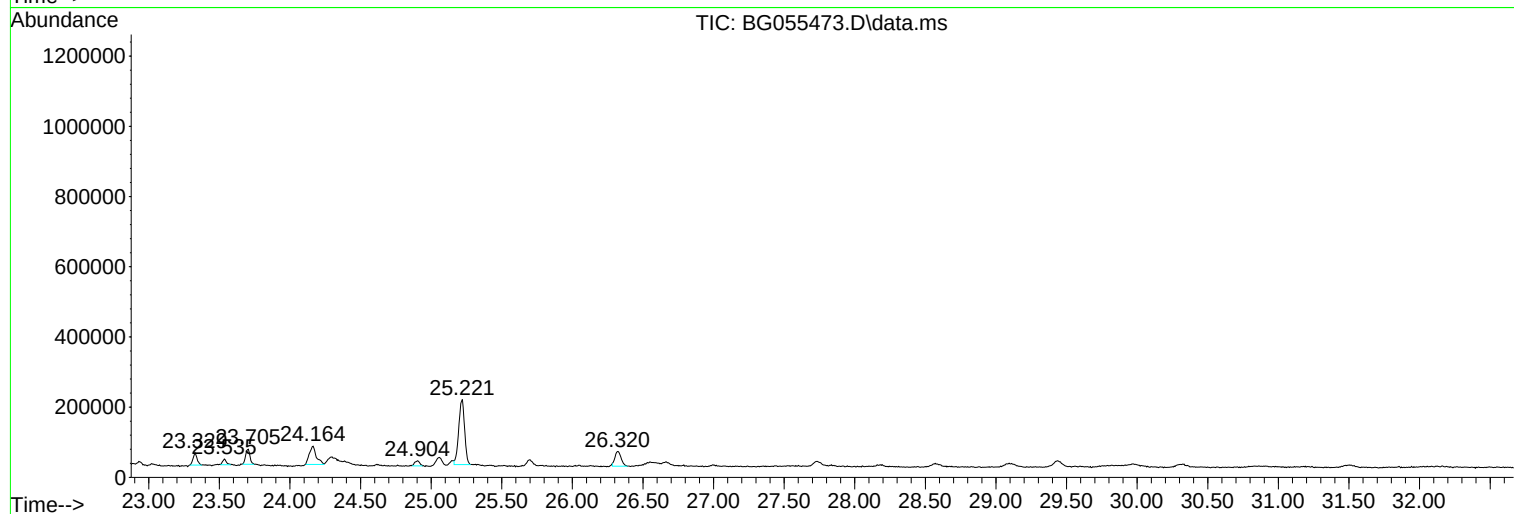
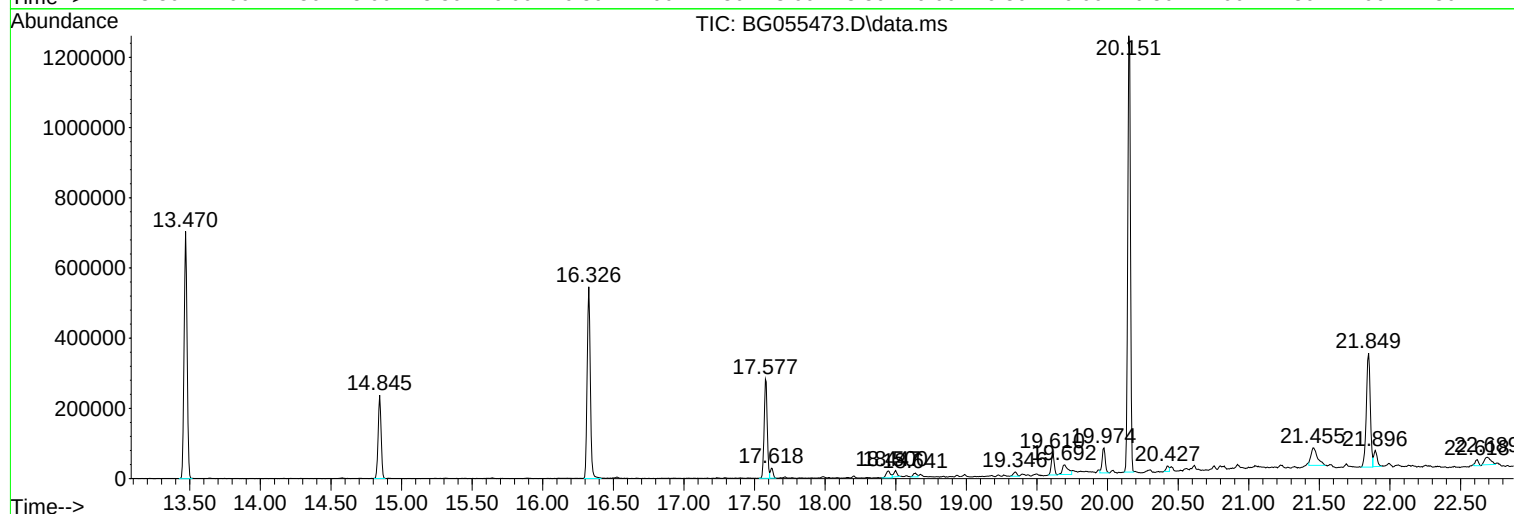
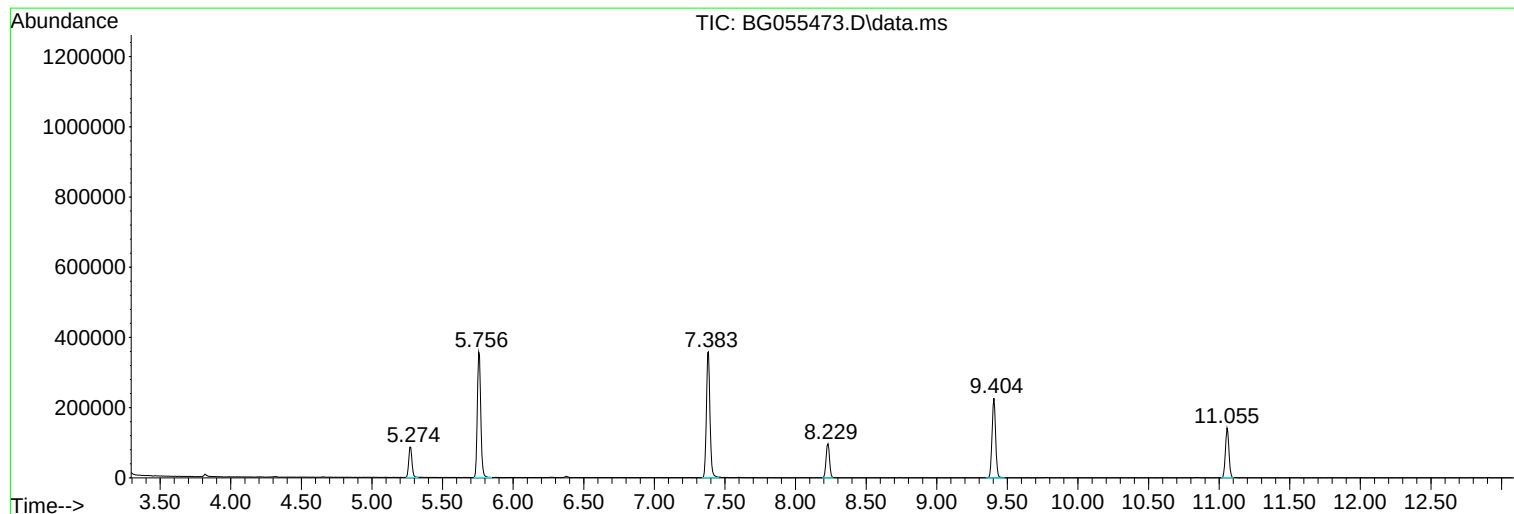
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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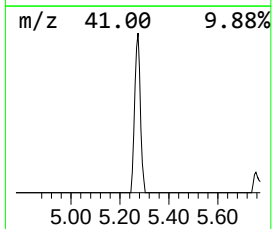
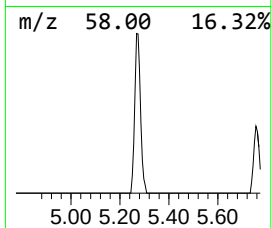
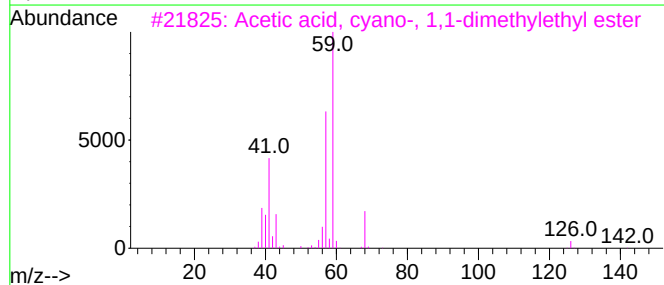
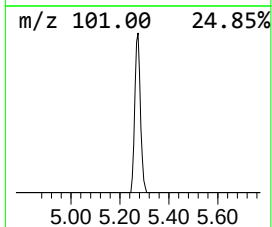
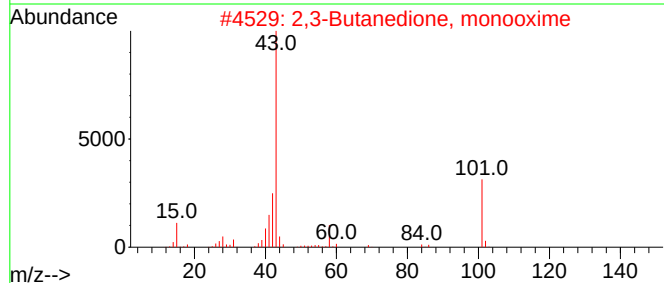
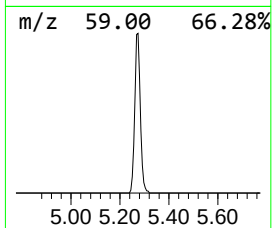
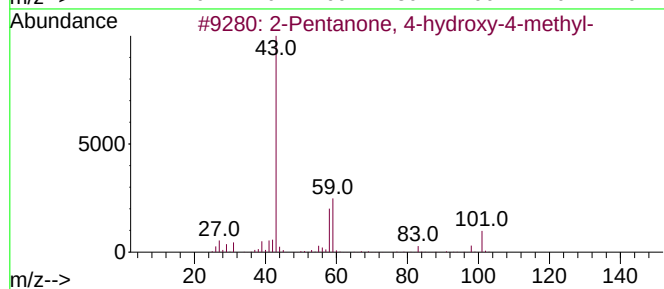
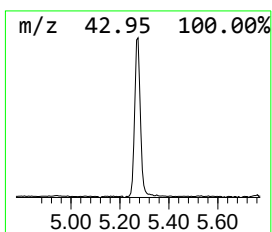
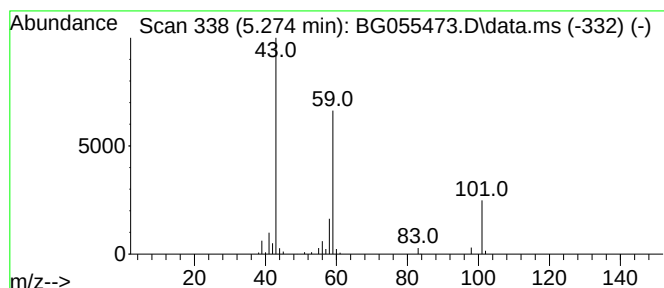
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.274	16.55 ng	136736	1,4-Dichlorobenzene-d4	8.229

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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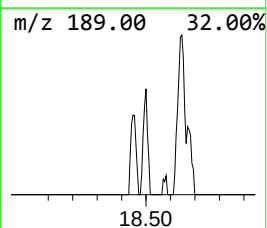
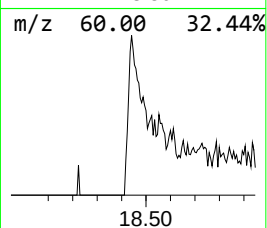
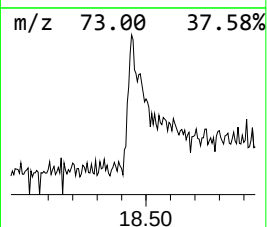
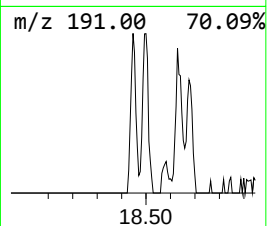
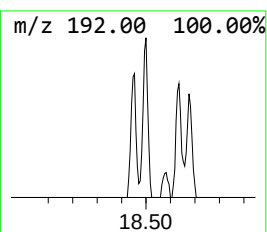
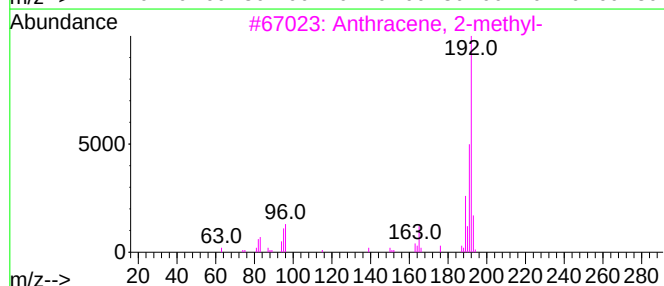
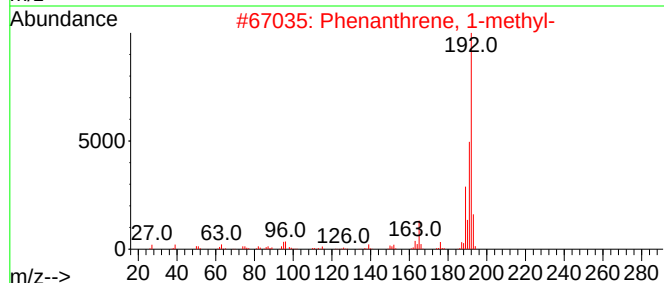
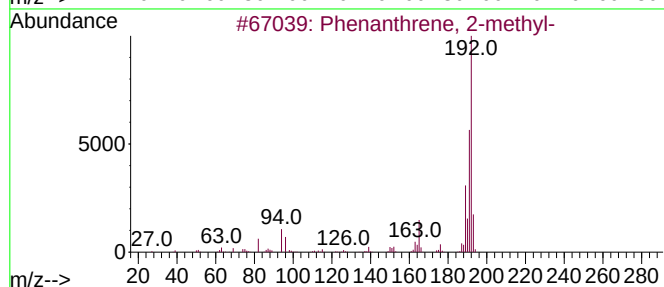
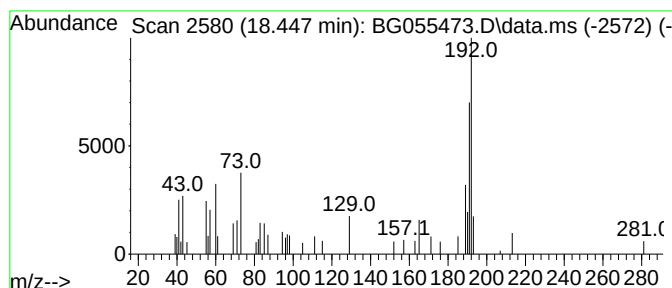
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Phenanthrene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.447	2.09 ng	45153	Phenanthrene-d10	17.577

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	64
2		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	58
3		Anthracene, 2-methyl-	192	C15H12	000613-12-7	58
4		Anthracene, 9-methyl-	192	C15H12	000779-02-2	53
5		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	53



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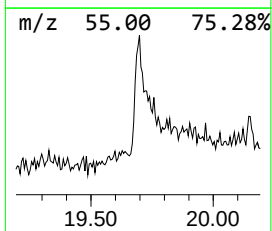
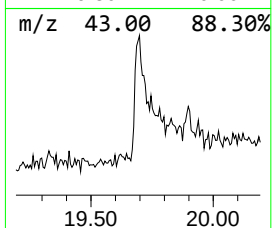
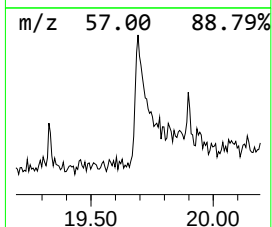
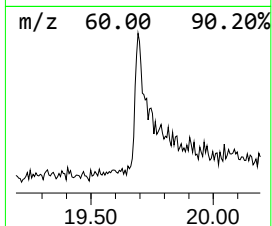
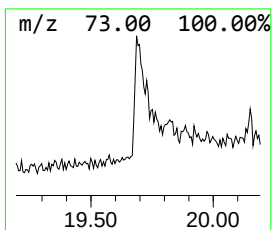
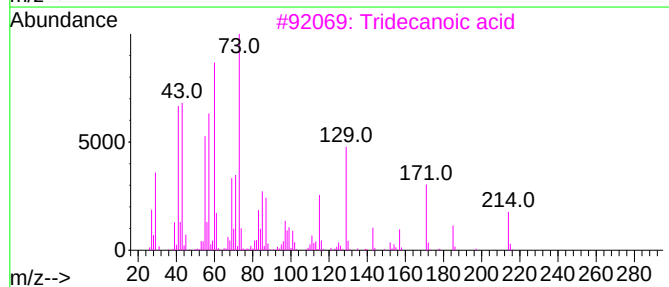
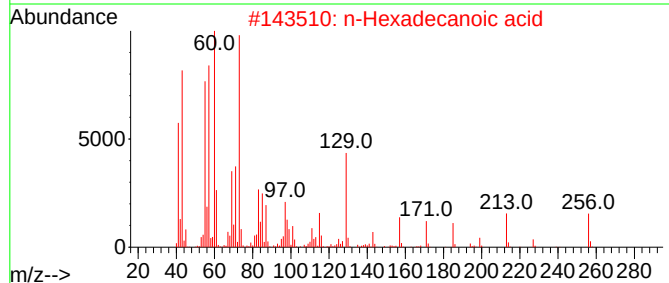
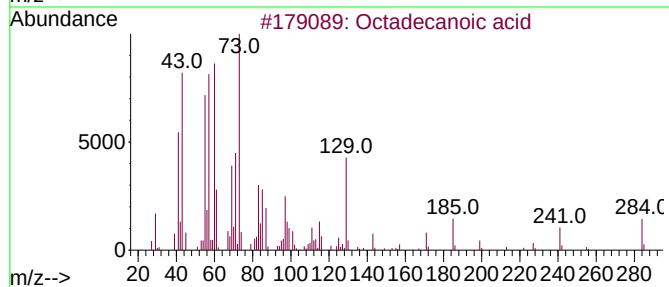
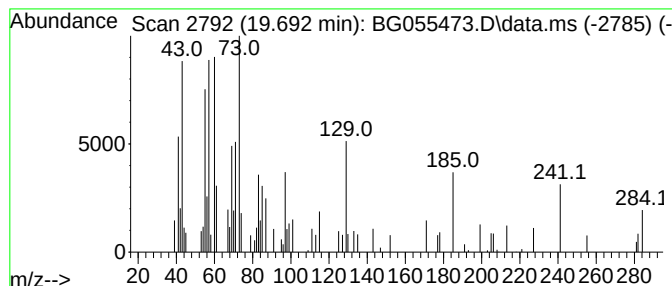
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.692	3.68 ng	79492	Phenanthrene-d10	17.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3			Tridecanoic acid	214	C13H26O2	000638-53-9	72
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	59



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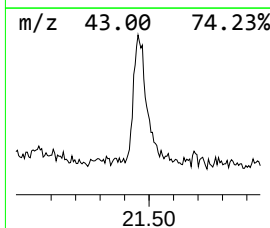
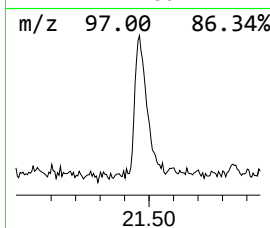
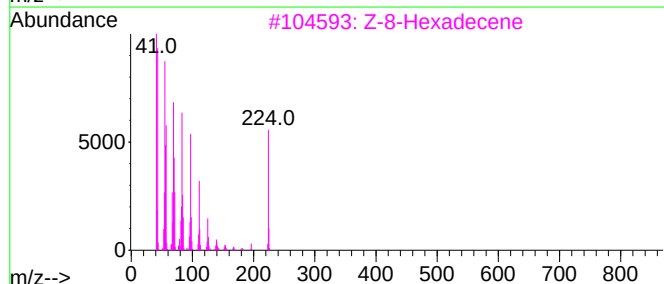
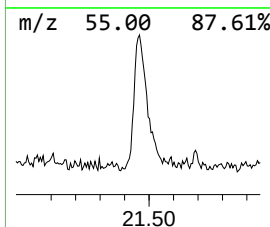
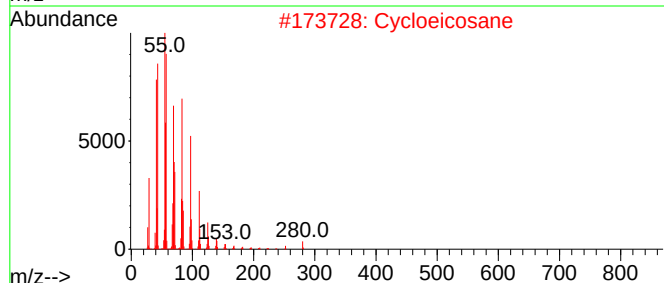
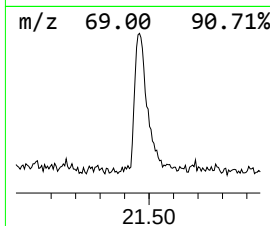
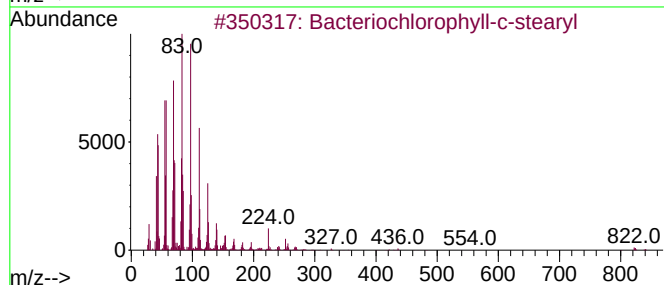
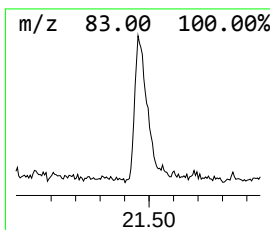
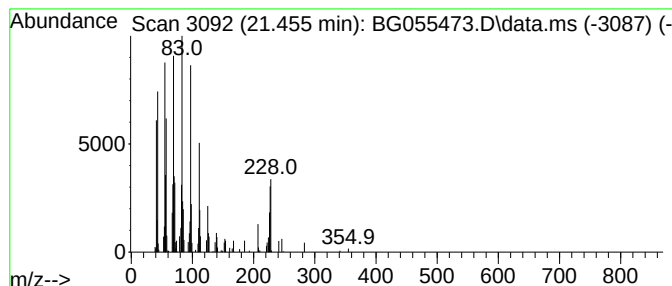
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Bacteriochlorophyll-c-stearyl Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.455	5.00 ng	157407	Chrysene-d12	21.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	70
2			Cycloeicosane	280	C20H40	000296-56-0	64
3			Z-8-Hexadecene	224	C16H32	1000130-87-5	62
4			1-Nonadecene	266	C19H38	018435-45-5	60
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	60



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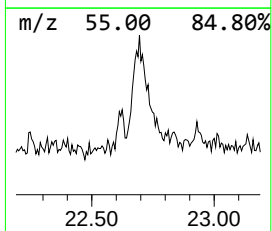
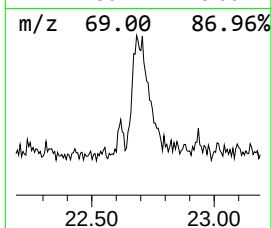
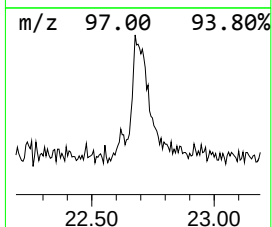
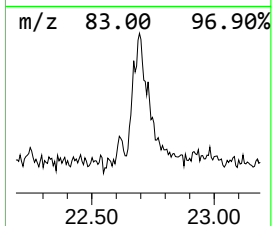
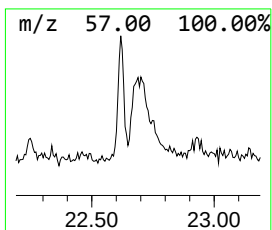
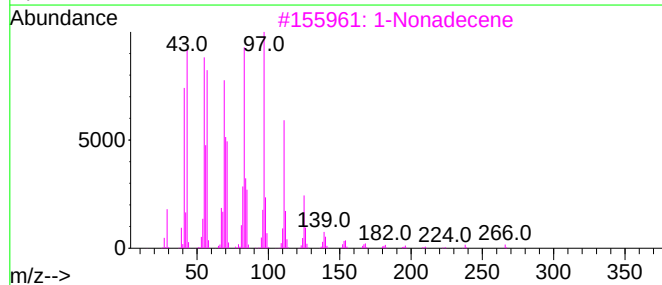
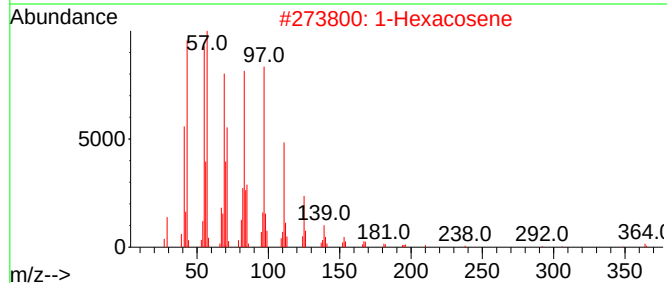
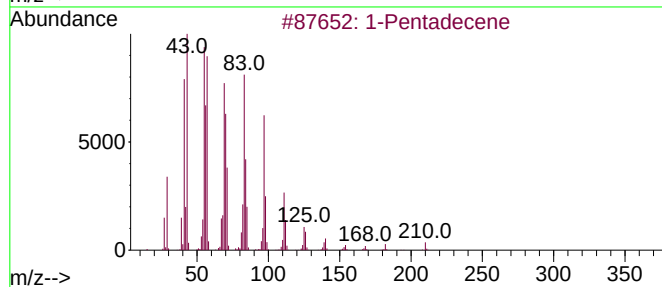
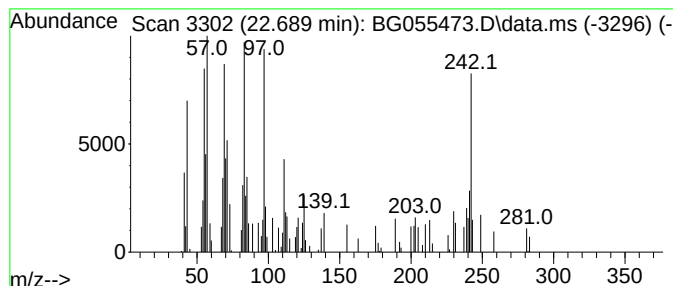
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Pentadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.689	2.18 ng	68591	Chrysene-d12	21.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecene			210	C15H30	013360-61-7	83
2	1-Hexacosene			364	C26H52	018835-33-1	64
3	1-Nonadecene			266	C19H38	018435-45-5	64
4	1-Hexadecanethiol			258	C16H34S	002917-26-2	60
5	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	58



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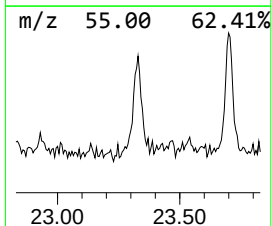
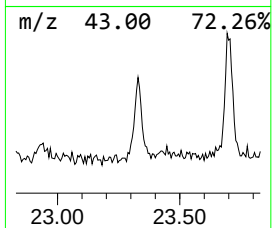
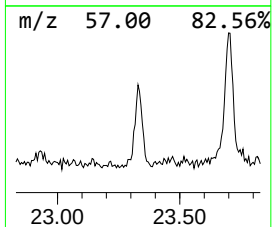
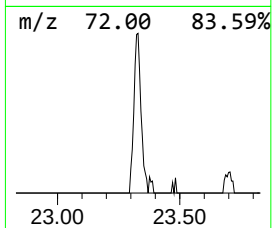
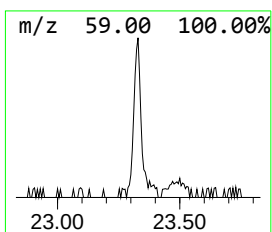
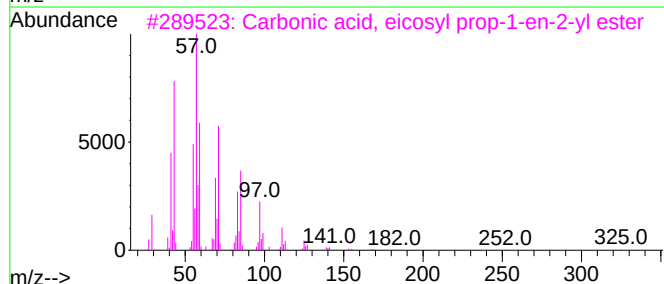
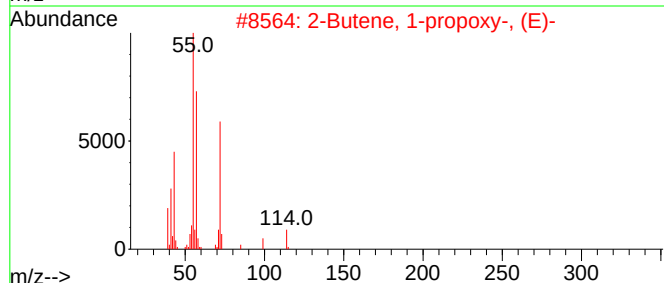
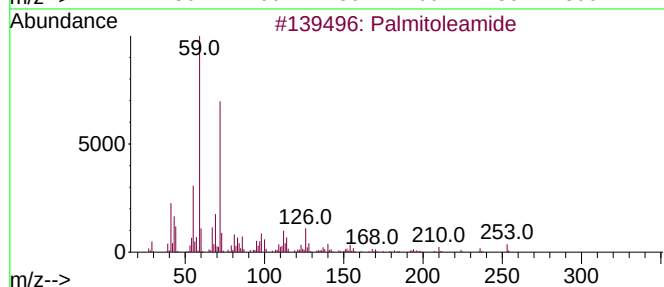
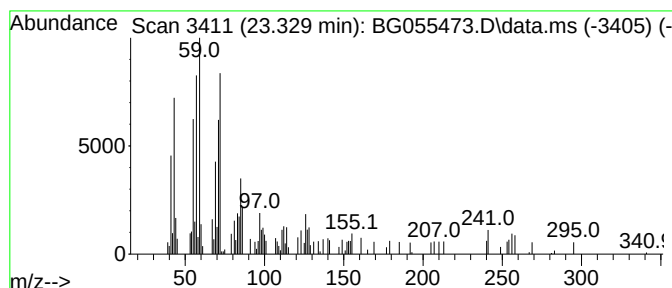
Instrument :
BNA_G
ClientSampleId :
TP-O

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Palmitoleamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.329	2.17 ng	68209	Chrysene-d12	21.849	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palmitoleamide	253	C16H31NO	106010-22-4	60
2	2-Butene, 1-propoxy-, (E)-	114	C7H14O	056052-71-2	25
3	Carbonic acid, eicosyl prop-1-en...	382	C24H46O3	1000383-10-8	25
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	18
5	2-Butene, 1-butoxy-, (E)-	128	C8H16O	056052-72-3	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110522\
Data File : BG055473.D
Acq On : 5 Nov 2022 16:48
Operator : CG/JU
Sample : N5418-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-O

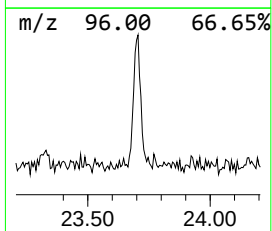
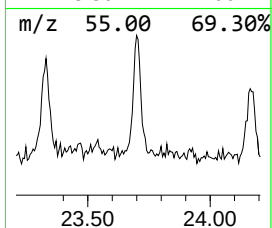
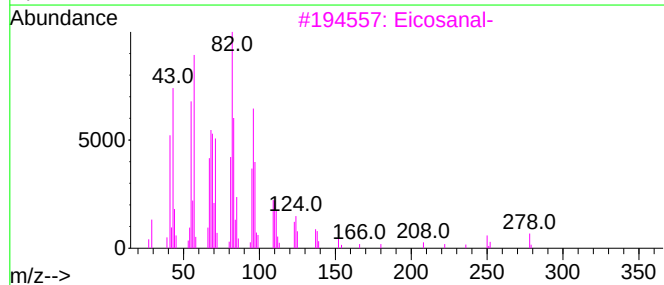
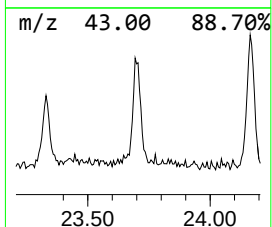
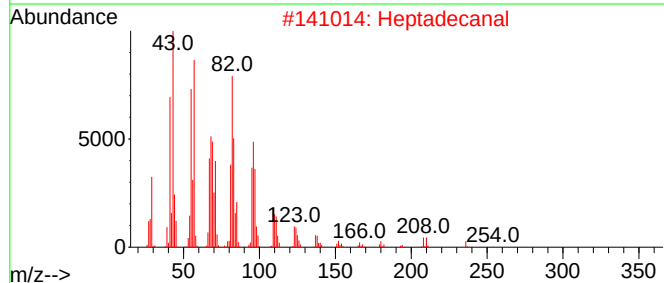
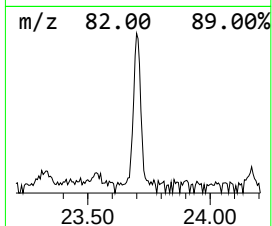
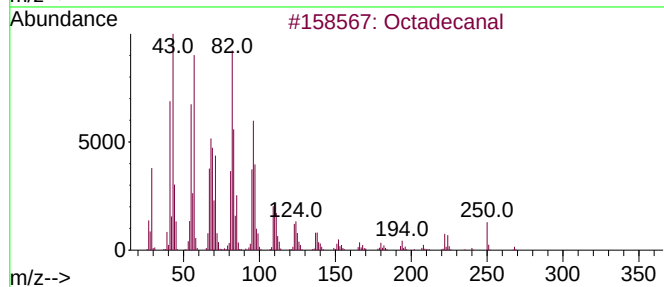
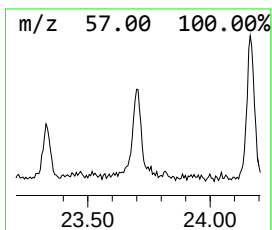
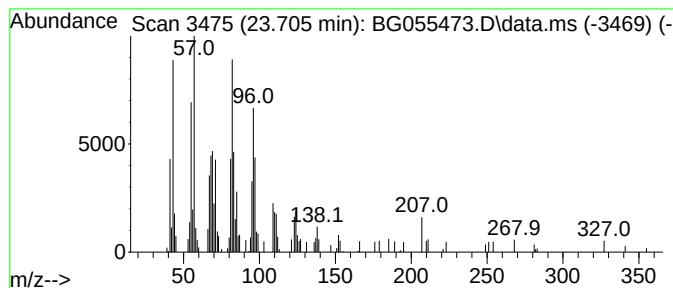
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.705	3.34 ng	89159	Perylene-d12	25.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal			268	C18H36O	000638-66-4	91
2	Heptadecanal			254	C17H34O	1000376-70-0	91
3	Eicosanal-			296	C20H40O	002400-66-0	91
4	Tetracosanal			352	C24H48O	057866-08-7	91
5	Hexadecanal			240	C16H32O	000629-80-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110522\
Data File : BG055473.D
Acq On : 5 Nov 2022 16:48
Operator : CG/JU
Sample : N5418-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-O

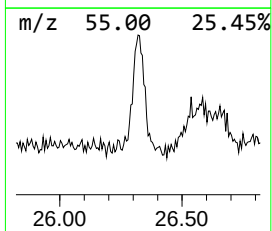
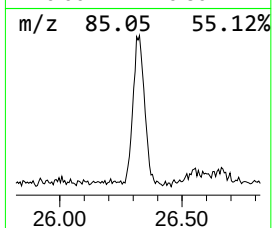
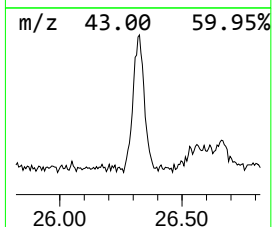
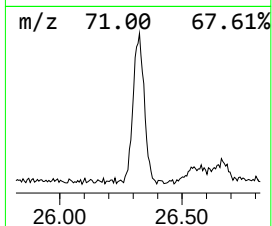
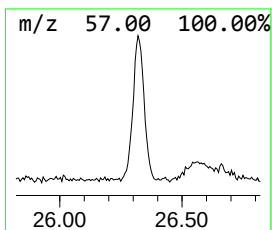
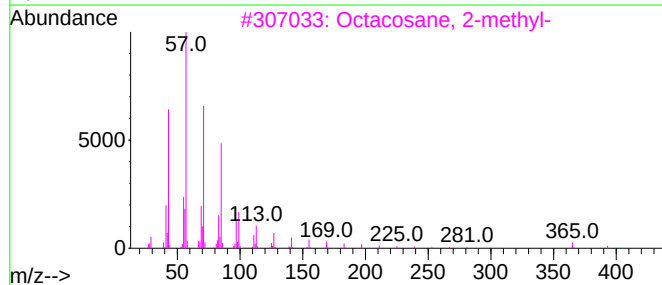
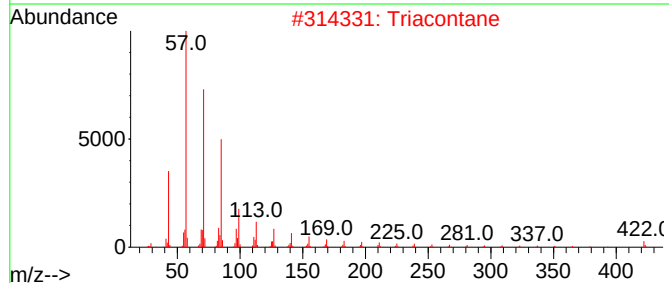
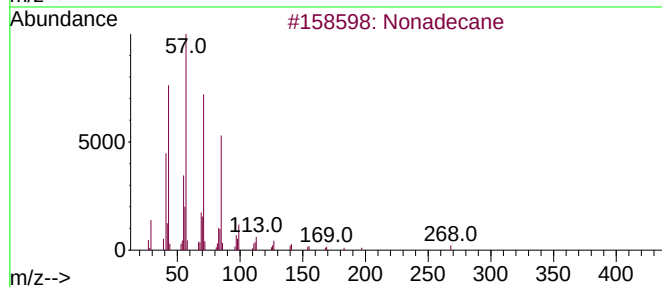
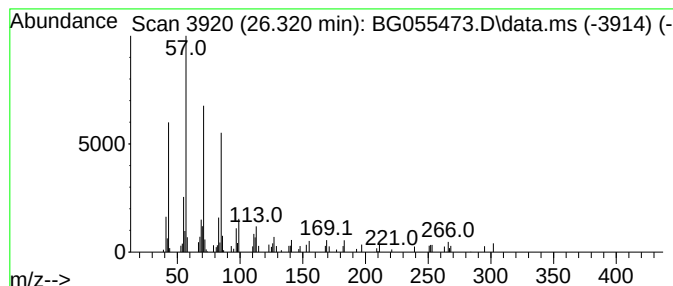
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.320	4.84 ng	129082	Perylene-d12	25.221

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	91
2			Triacontane	422	C30H62	000638-68-6	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4			Octacosane	394	C28H58	000630-02-4	86
5			Eicosane, 2-methyl-	296	C21H44	001560-84-5	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110522\
Data File : BG055473.D
Acq On : 5 Nov 2022 16:48
Operator : CG/JU
Sample : N5418-16
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-O

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.274	16.6	ng	136736	1	8.229	165241	20.0
Phenanthrene, 2...	18.447	2.1	ng	45153	4	17.577	432493	20.0
Octadecanoic acid	19.692	3.7	ng	79492	4	17.577	432493	20.0
Bacteriochlorop...	21.455	5.0	ng	157407	5	21.849	629643	20.0
1-Pentadecene	22.689	2.2	ng	68591	5	21.849	629643	20.0
Palmitoleamide	23.329	2.2	ng	68209	5	21.849	629643	20.0
Octadecanal	23.705	3.3	ng	89159	6	25.221	533797	20.0
Nonadecane	26.320	4.8	ng	129082	6	25.221	533797	20.0