

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057836.D
 Acq On : 23 Jun 2023 10:38
 Operator : CG/JU
 Sample : 03238-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-4B

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.491	402	409	417	rBV	300956	453423	15.19%	3.433%
2	7.077	672	679	690	rVB	184678	305578	10.23%	2.314%
3	7.923	816	823	833	rBV	112704	190992	6.40%	1.446%
4	9.081	1010	1020	1030	rBV	417789	728628	24.40%	5.517%
5	10.726	1292	1300	1308	rBV	166145	294439	9.86%	2.229%
6	13.182	1710	1718	1726	rVB	1117250	1662784	55.69%	12.590%
7	14.557	1945	1952	1962	rBV	299600	464179	15.55%	3.515%
8	15.914	2177	2183	2188	rBV	120570	174907	5.86%	1.324%
9	16.043	2195	2205	2228	rVB	1141176	1838159	61.56%	13.918%
10	16.707	2311	2318	2319	rBV6	19473	32972	1.10%	0.250%
11	17.301	2413	2419	2427	rVB	434240	651548	21.82%	4.933%
12	17.882	2510	2518	2519	rBV4	26750	52061	1.74%	0.394%
13	18.188	2565	2570	2582	rBV	124445	212747	7.13%	1.611%
14	19.322	2755	2763	2776	rBV2	96191	239657	8.03%	1.815%
15	19.463	2784	2787	2796	rVB2	59480	92480	3.10%	0.700%
16	19.921	2859	2865	2871	rVB	2245757	2985728	100.00%	22.608%
17	20.309	2925	2931	2941	rVB	106477	215897	7.23%	1.635%
18	20.515	2960	2966	2974	rBV2	106796	249490	8.36%	1.889%
19	21.155	3068	3075	3081	rBV	114797	262647	8.80%	1.989%
20	21.214	3081	3085	3093	rVB3	30883	66067	2.21%	0.500%
21	21.290	3094	3098	3104	rVB	36785	53817	1.80%	0.407%
22	21.555	3137	3143	3152	rVB2	426022	692493	23.19%	5.244%
23	22.101	3230	3236	3246	rVB2	93772	238936	8.00%	1.809%
24	23.217	3420	3426	3438	rVB2	91722	249016	8.34%	1.886%
25	24.710	3670	3680	3694	rVB	268888	798049	26.73%	6.043%

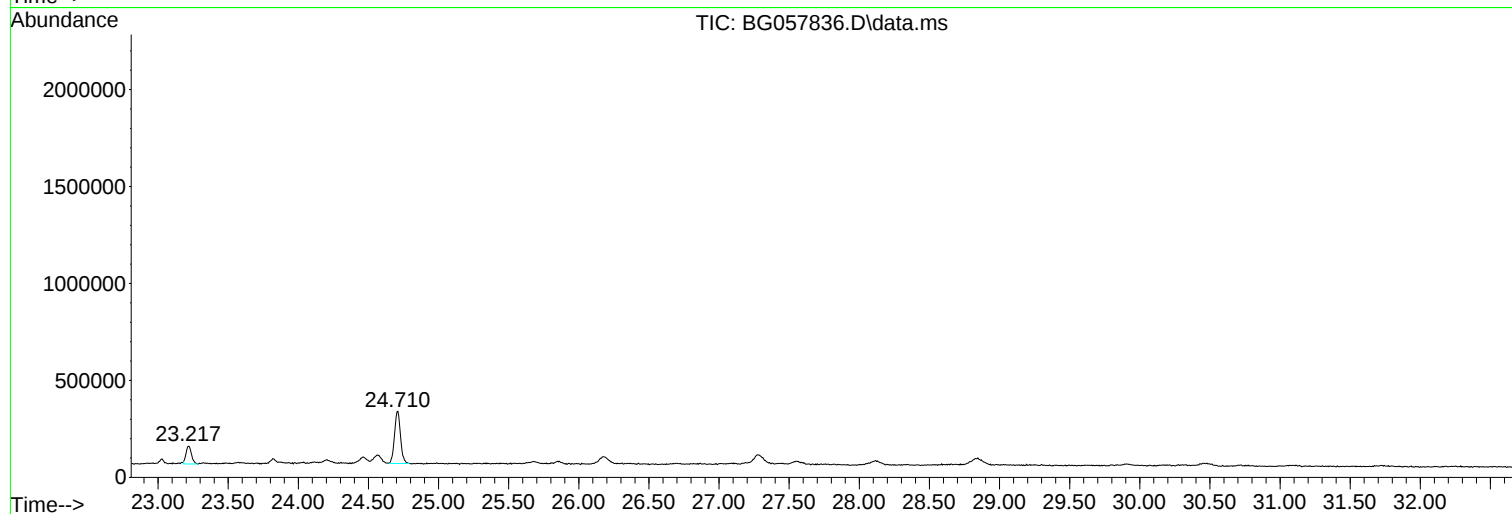
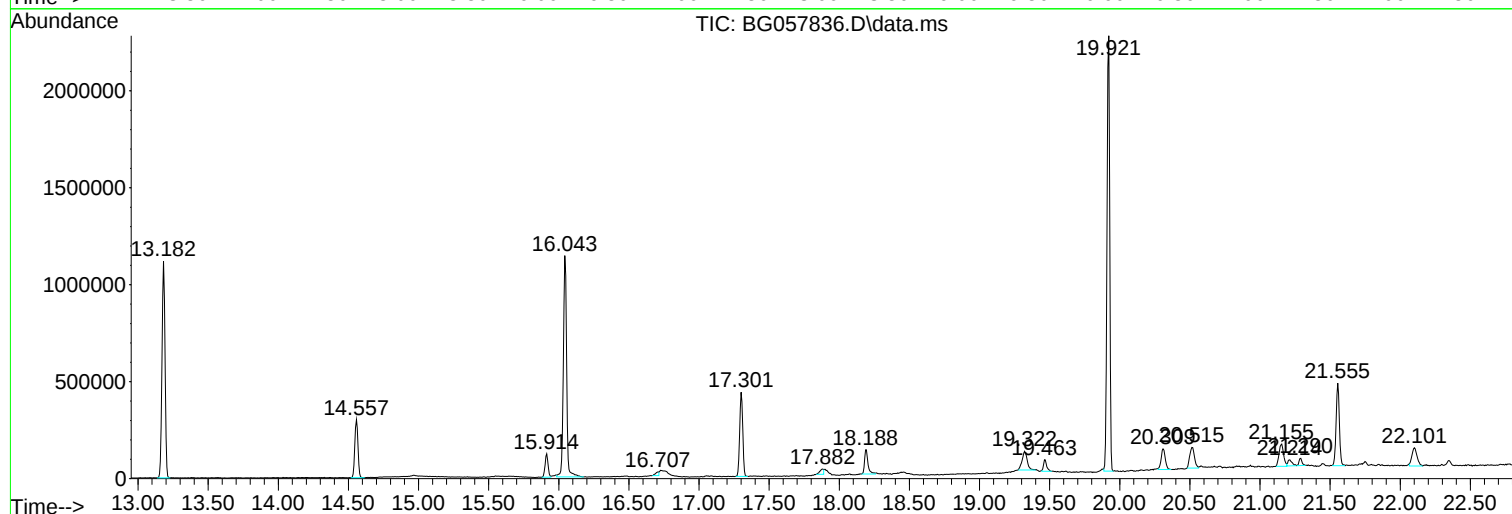
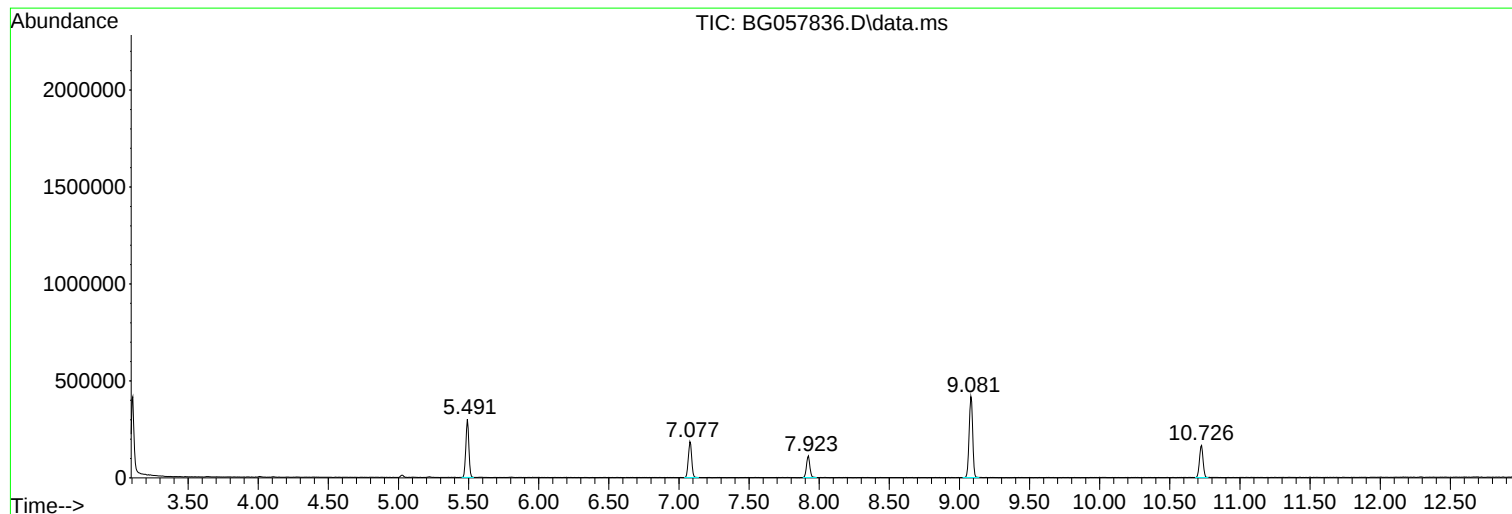
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Instrument :
BNA_G
ClientSampleId :
MW-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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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Instrument :
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ClientSampleId :
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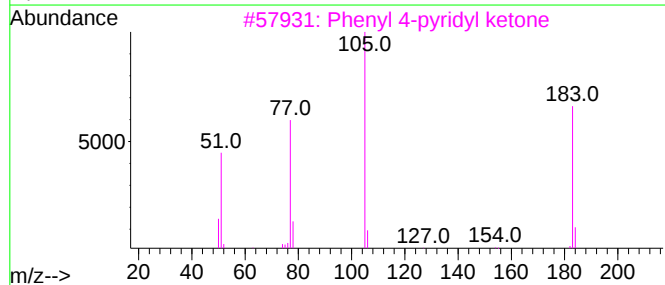
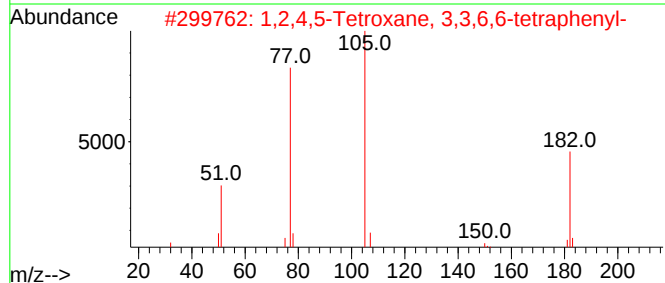
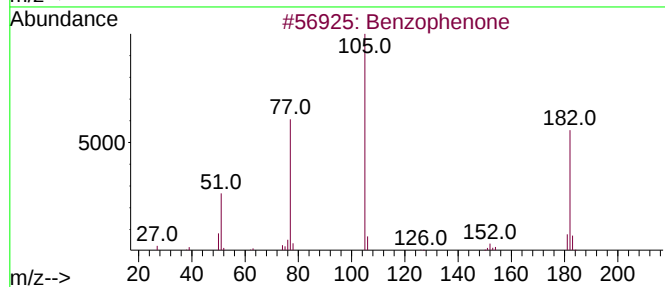
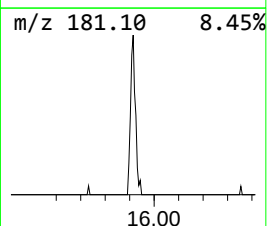
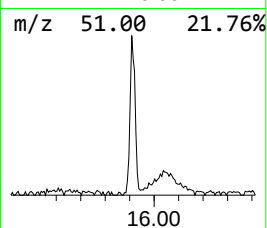
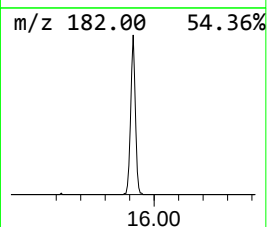
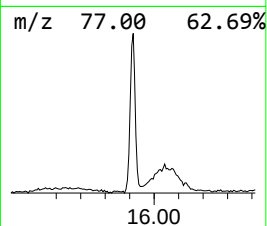
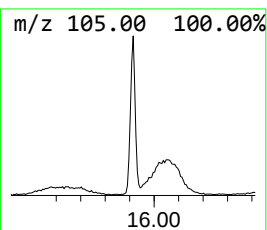
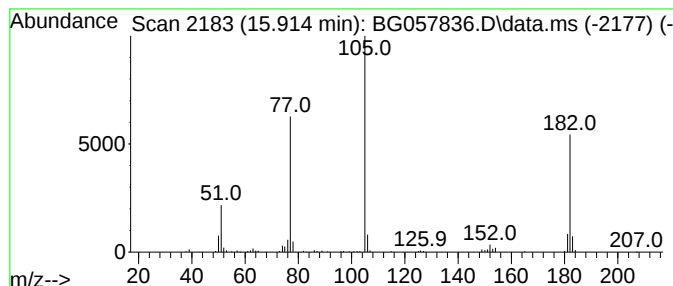
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	7.54 ng	174907	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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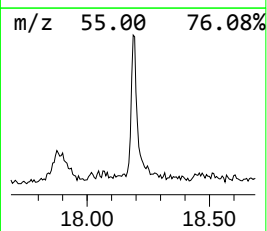
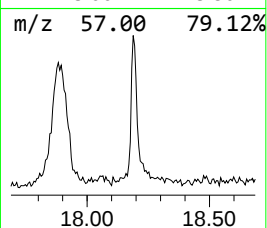
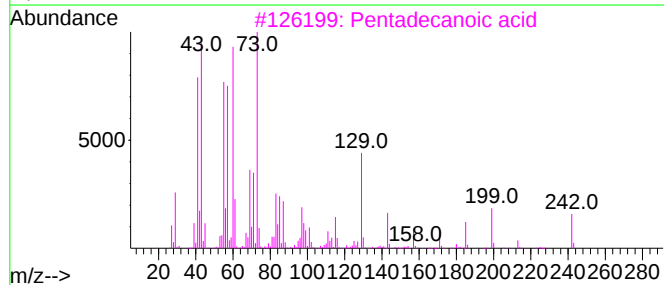
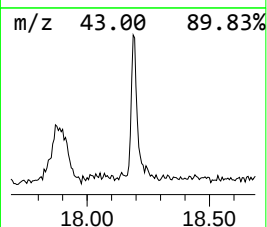
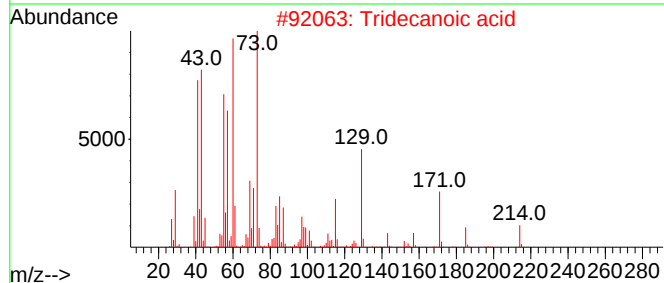
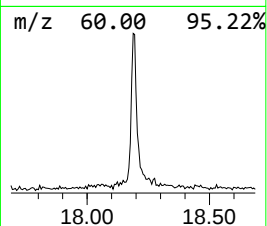
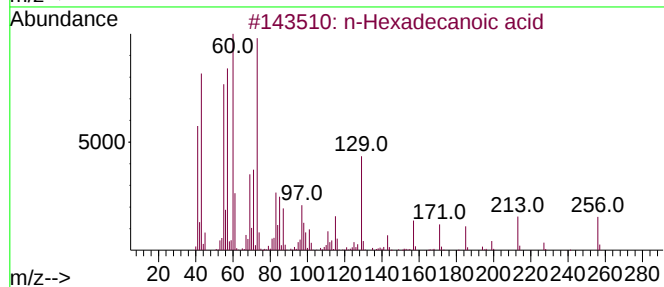
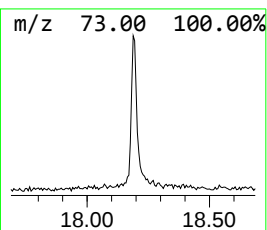
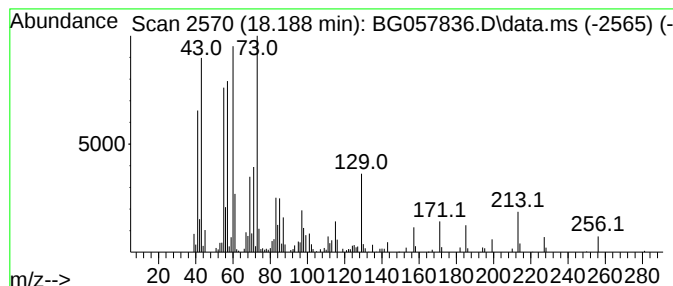
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	6.53 ng	212747	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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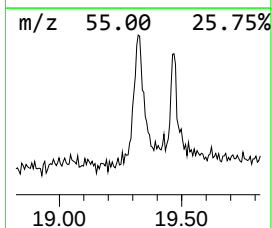
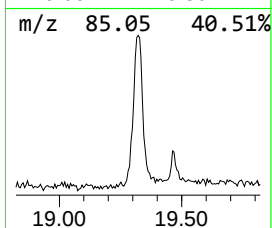
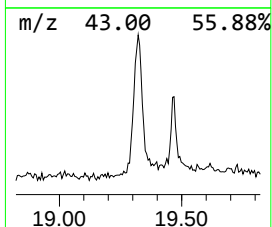
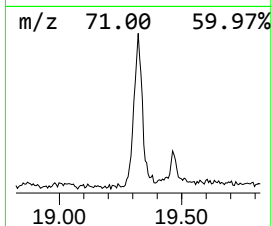
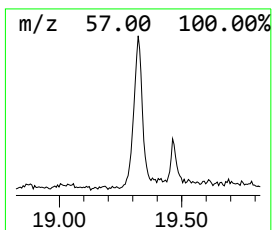
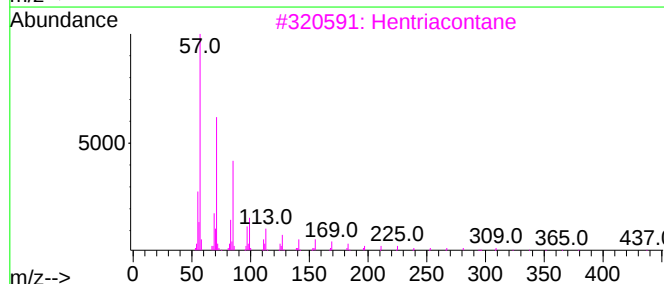
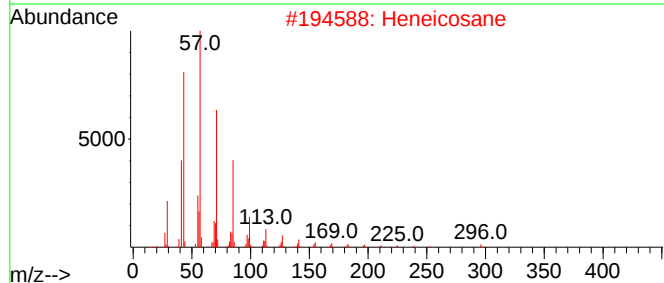
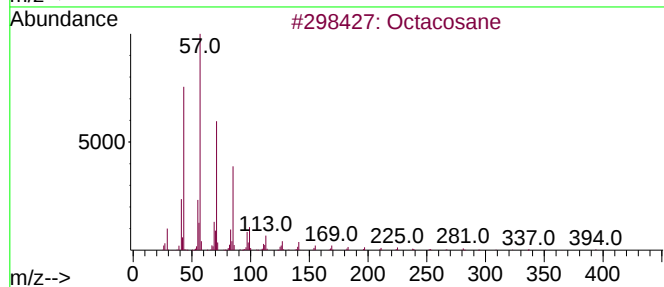
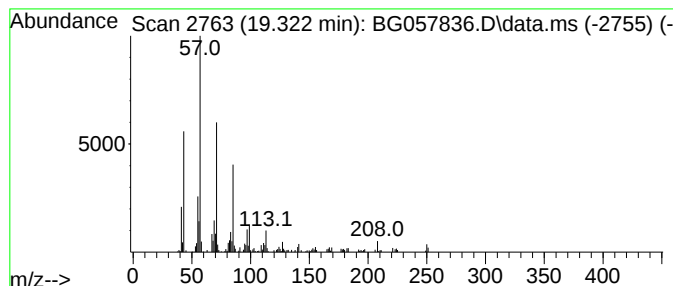
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.322	7.36 ng	239657	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	90
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hentriacontane	437	C31H64	000630-04-6	87
4			Heptacosane	380	C27H56	000593-49-7	83
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83



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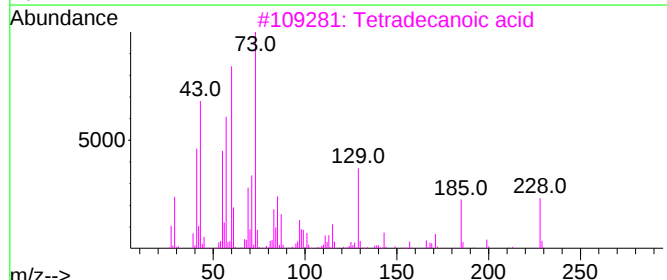
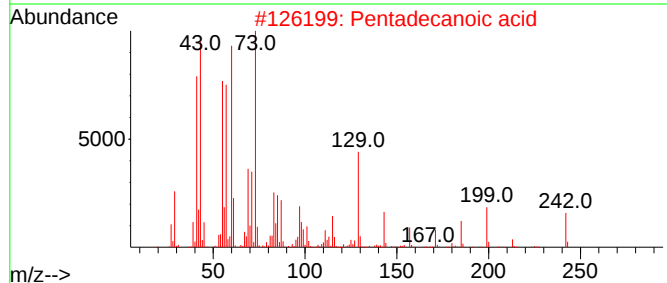
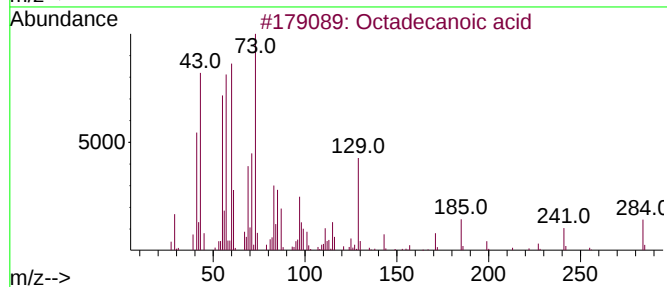
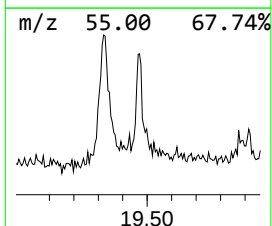
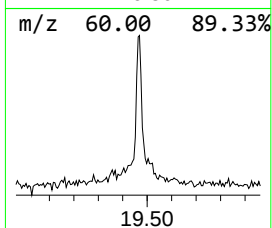
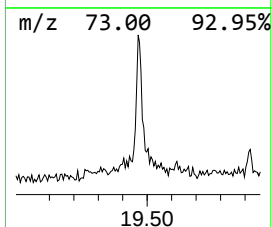
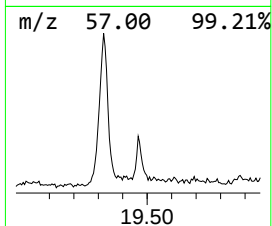
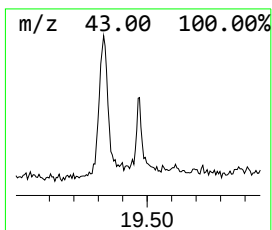
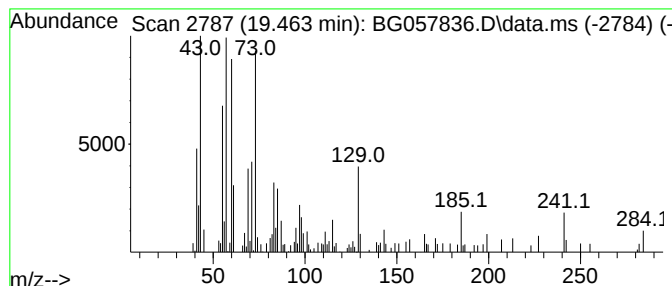
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	2.67 ng	92480	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			n-Decanoic acid	172	C10H20O2	000334-48-5	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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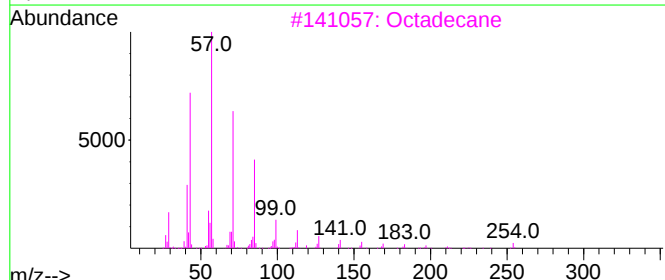
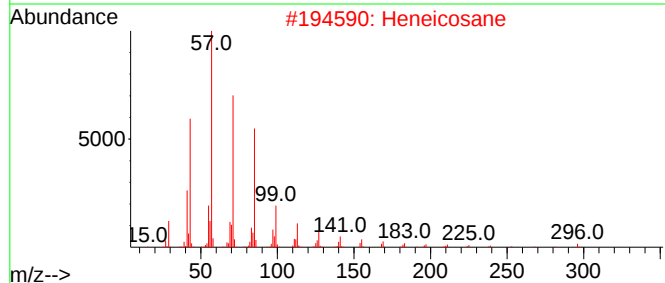
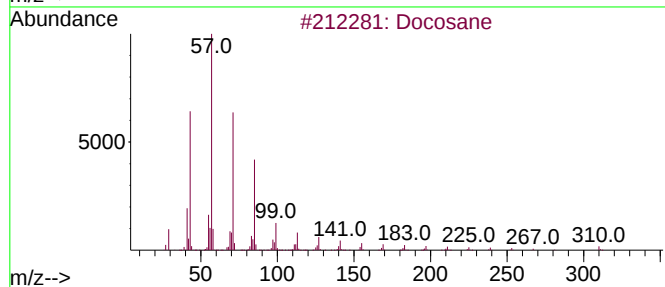
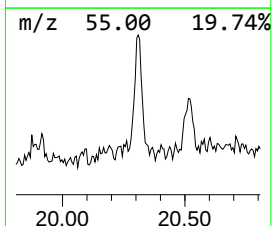
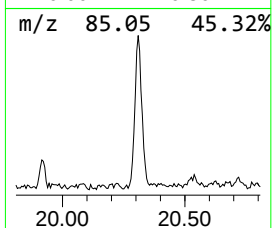
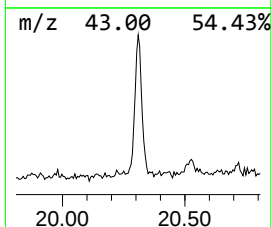
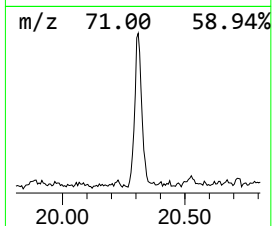
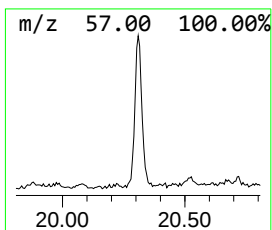
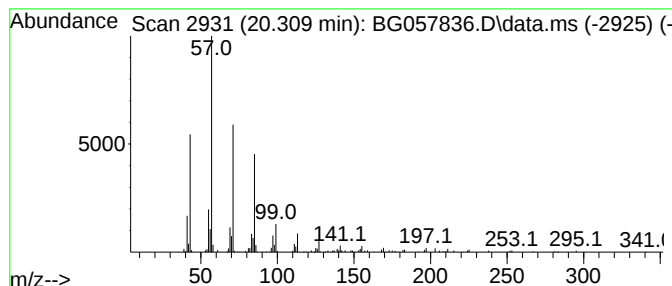
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Peak Number 5 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.309	6.24 ng	215897	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	91
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octadecane	254	C18H38	000593-45-3	87
4			Heptadecane	240	C17H36	000629-78-7	86
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



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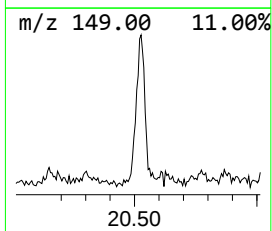
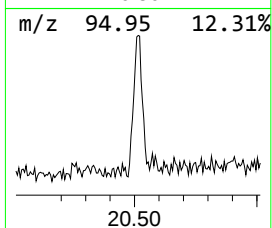
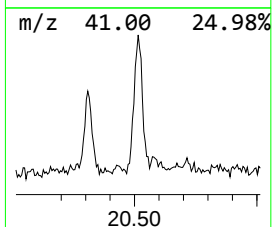
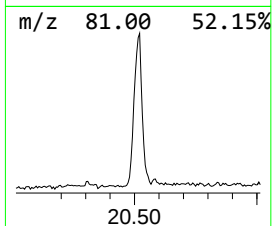
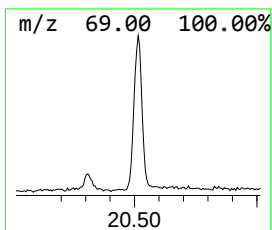
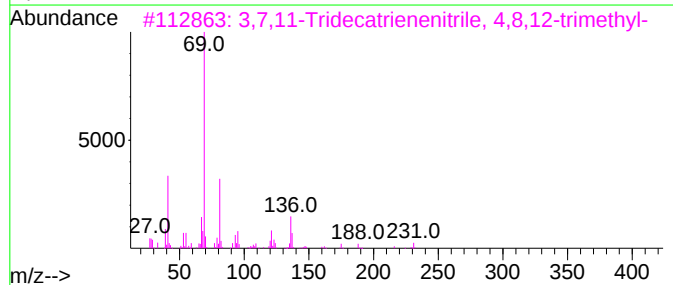
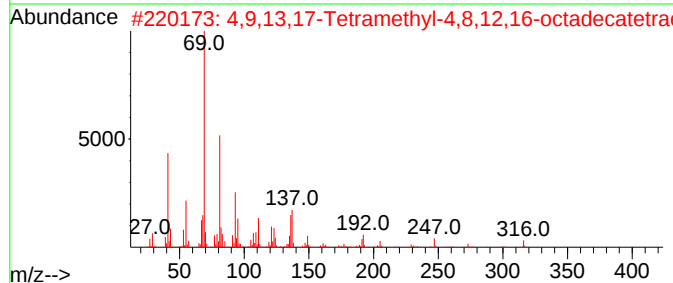
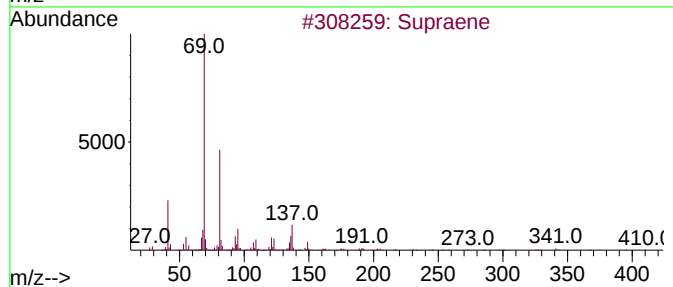
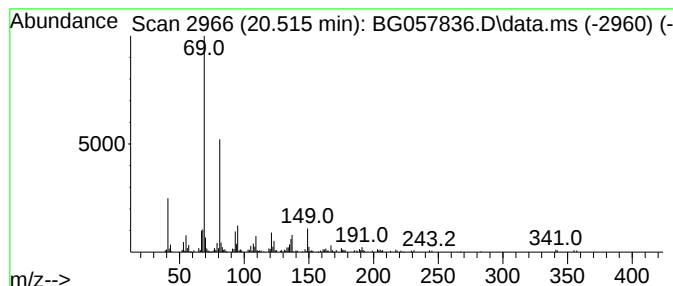
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.515	7.21 ng	249490	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	83
2			4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
3			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
5			4-Oxo-.beta.-damascone	206	C13H18O2	053398-08-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057836.D
Acq On : 23 Jun 2023 10:38
Operator : CG/JU
Sample : 03238-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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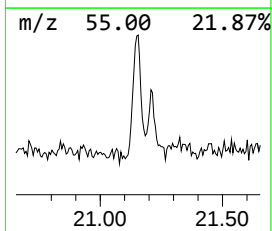
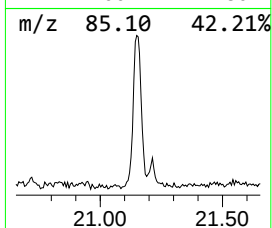
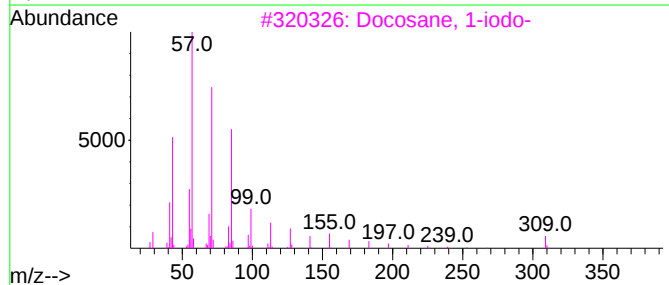
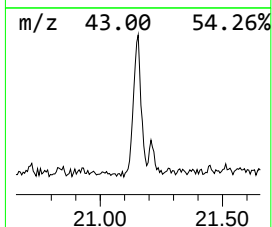
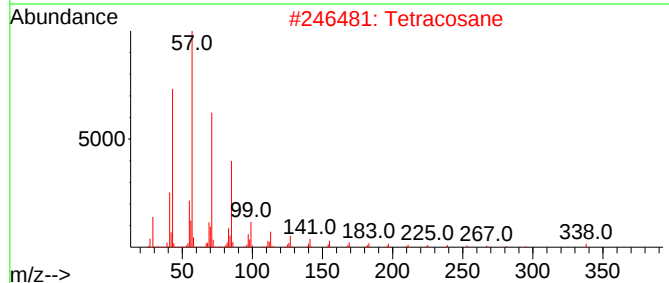
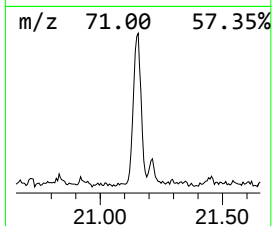
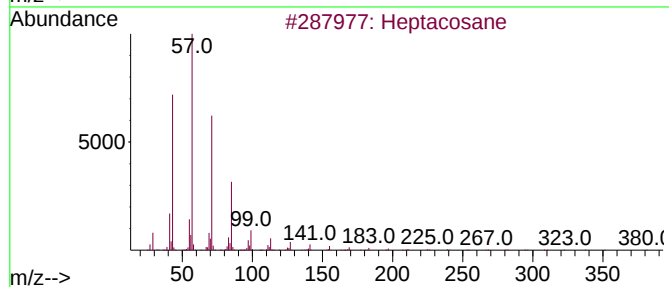
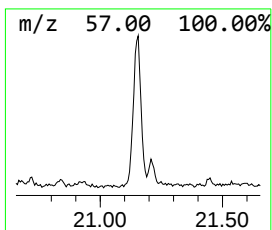
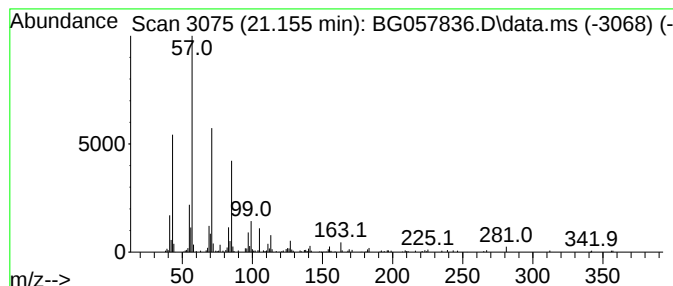
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.155	7.59 ng	262647	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Tetracosane	338	C24H50	000646-31-1	90
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	86
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	86
5			Heneicosane	296	C21H44	000629-94-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057836.D
Acq On : 23 Jun 2023 10:38
Operator : CG/JU
Sample : 03238-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4B

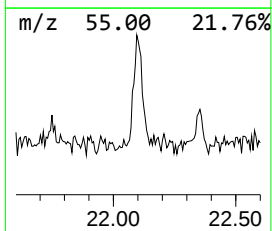
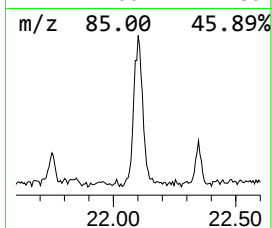
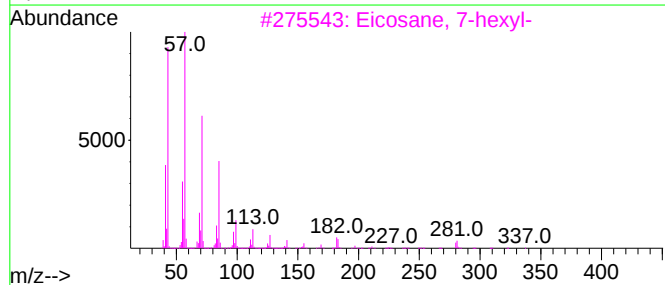
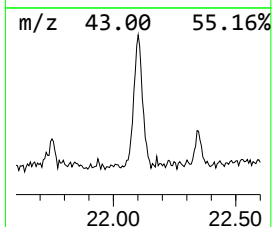
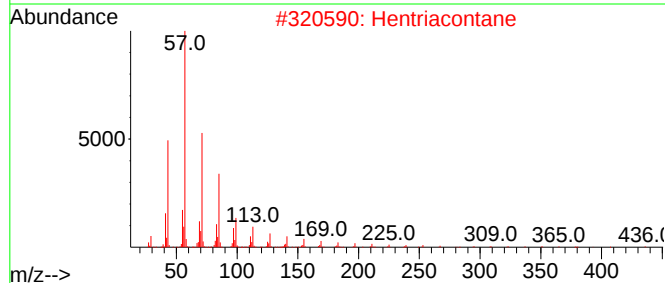
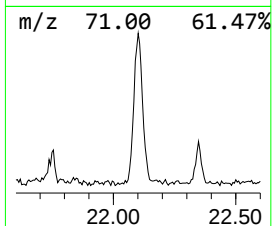
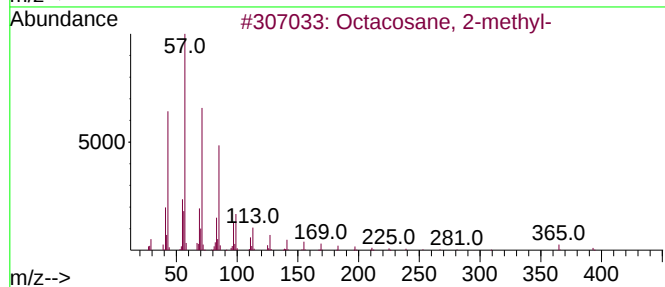
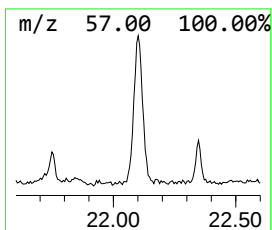
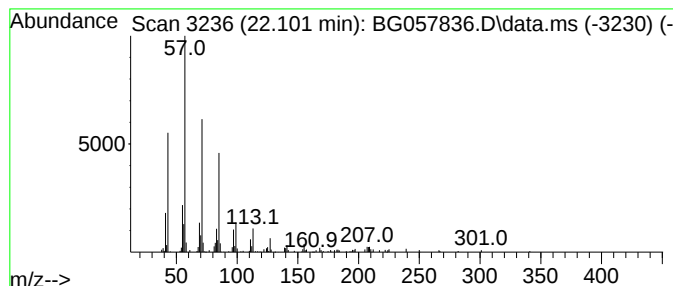
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.101	6.90 ng	238936	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
2			Hentriacontane	437	C31H64	000630-04-6	87
3			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	86
5			4-Methylheneicosane	310	C22H46	025117-29-7	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057836.D
Acq On : 23 Jun 2023 10:38
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Sample : 03238-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

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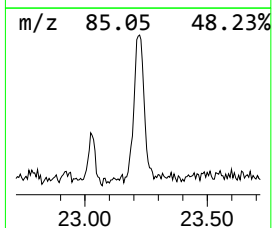
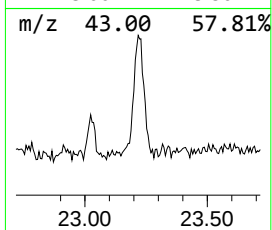
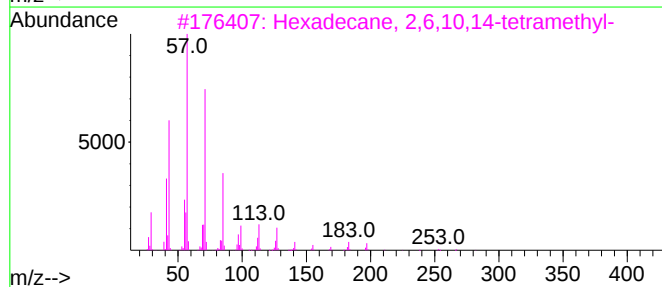
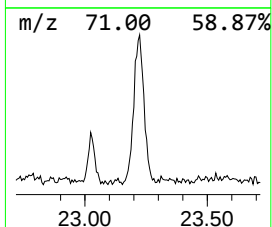
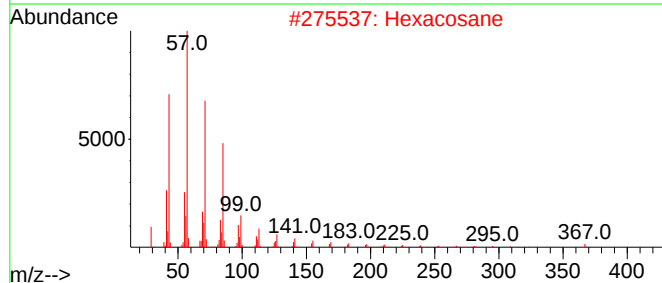
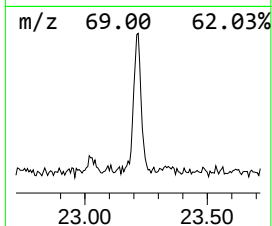
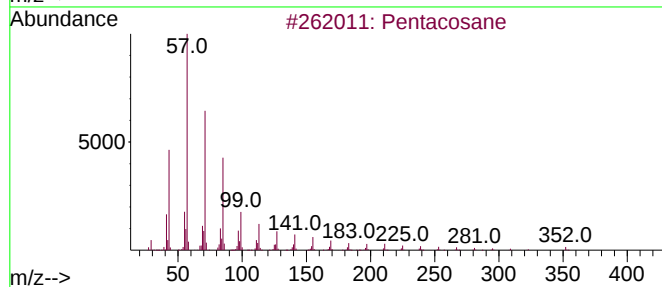
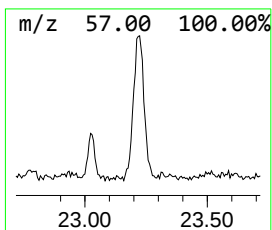
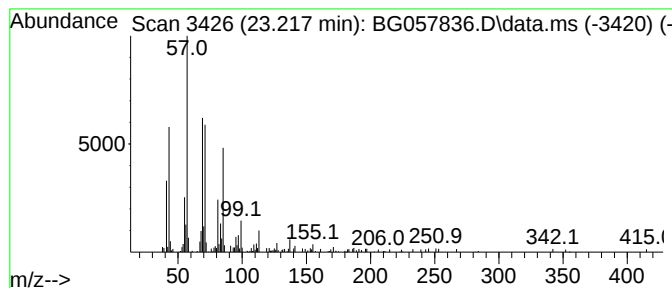
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.217	6.24 ng	249016	Perylene-d12	24.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	93
2			Hexacosane	366	C26H54	000630-01-3	90
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	89
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
5			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057836.D
Acq On : 23 Jun 2023 10:38
Operator : CG/JU
Sample : 03238-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.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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n-Hexadecanoic ...	18.188	6.5	ng	212747	4	17.301	651548	20.0
Octacosane	19.322	7.4	ng	239657	4	17.301	651548	20.0
Octadecanoic acid	19.463	2.7	ng	92480	5	21.555	692493	20.0
Docosane	20.309	6.2	ng	215897	5	21.555	692493	20.0
Supraene	20.515	7.2	ng	249490	5	21.555	692493	20.0
Heptacosane	21.155	7.6	ng	262647	5	21.555	692493	20.0
Octacosane, 2-m...	22.101	6.9	ng	238936	5	21.555	692493	20.0
Pentacosane	23.217	6.2	ng	249016	6	24.710	798049	20.0