

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
 Data File : BG060806.D
 Acq On : 6 Apr 2024 11:19
 Operator : MA/JU
 Sample : PB160028BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB160028BL

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060806.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	350	355	362	rBV	59555	84768	1.30%	0.326%
2	5.539	427	434	443	rBV	1211856	1851253	28.30%	7.127%
3	7.120	693	703	713	rBV	1280561	2117055	32.37%	8.151%
4	7.954	838	845	853	rVB	205877	349769	5.35%	1.347%
5	9.111	1032	1042	1050	rBV	689173	1224886	18.73%	4.716%
6	10.751	1314	1321	1330	rBV	289094	515323	7.88%	1.984%
7	13.213	1732	1740	1748	rBV	2021391	3152947	48.20%	12.139%
8	14.587	1966	1974	1985	rBV	511878	839291	12.83%	3.231%
9	16.074	2220	2227	2242	rBV	1901540	2991425	45.73%	11.517%
10	17.331	2434	2441	2450	rBV	854485	1267461	19.38%	4.880%
11	19.435	2793	2799	2803	rBV	53861	67909	1.04%	0.261%
12	19.670	2835	2839	2844	rVB	140045	163357	2.50%	0.629%
13	19.958	2881	2888	2896	rBV	4747493	6541096	100.00%	25.184%
14	20.716	3013	3017	3022	rVB	124329	137937	2.11%	0.531%
15	21.597	3160	3167	3177	rVB	900475	1468856	22.46%	5.655%
16	23.130	3423	3428	3437	rVB2	82930	161403	2.47%	0.621%
17	23.935	3559	3565	3573	rVB2	99572	220045	3.36%	0.847%
18	24.734	3692	3701	3713	rVB	542225	1515702	23.17%	5.836%
19	24.875	3718	3725	3733	rBV	118972	307929	4.71%	1.186%
20	26.009	3909	3918	3929	rVB2	112721	352433	5.39%	1.357%
21	27.361	4137	4148	4159	rVB	103681	358981	5.49%	1.382%
22	28.994	4414	4426	4437	rVB4	66946	283874	4.34%	1.093%

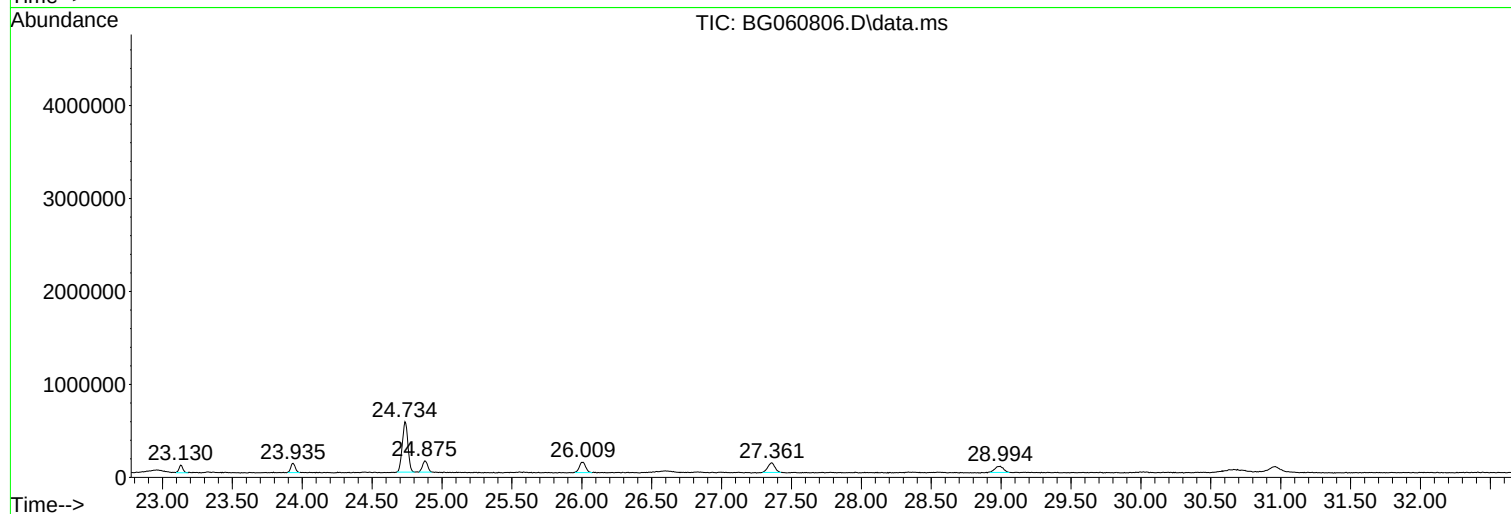
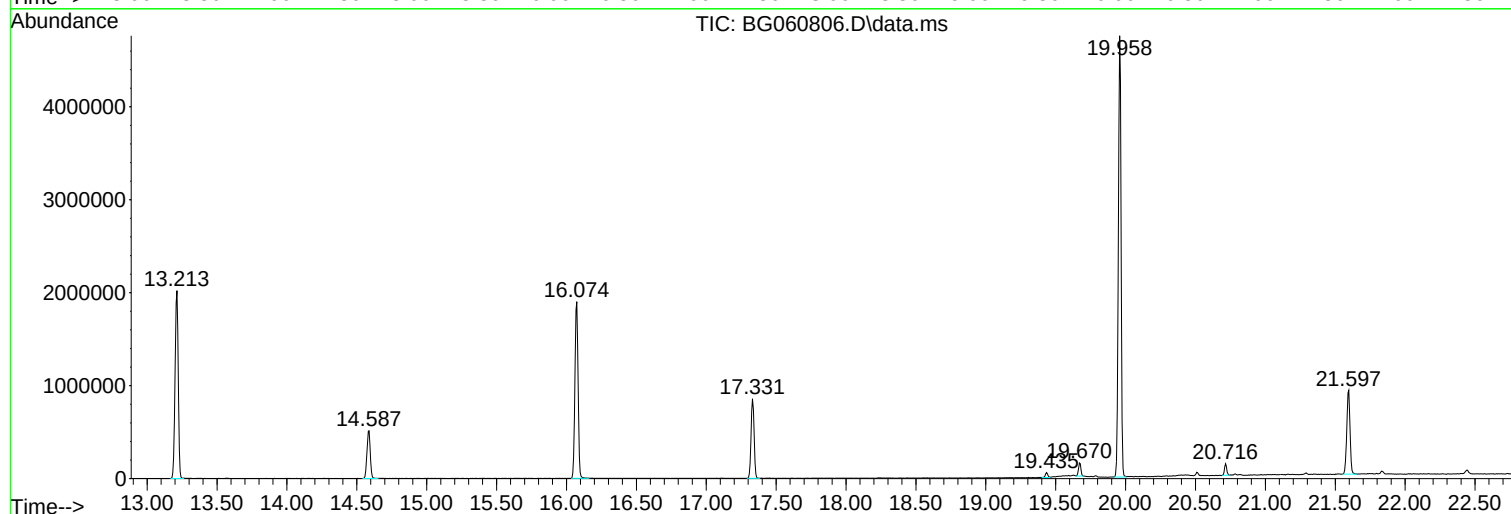
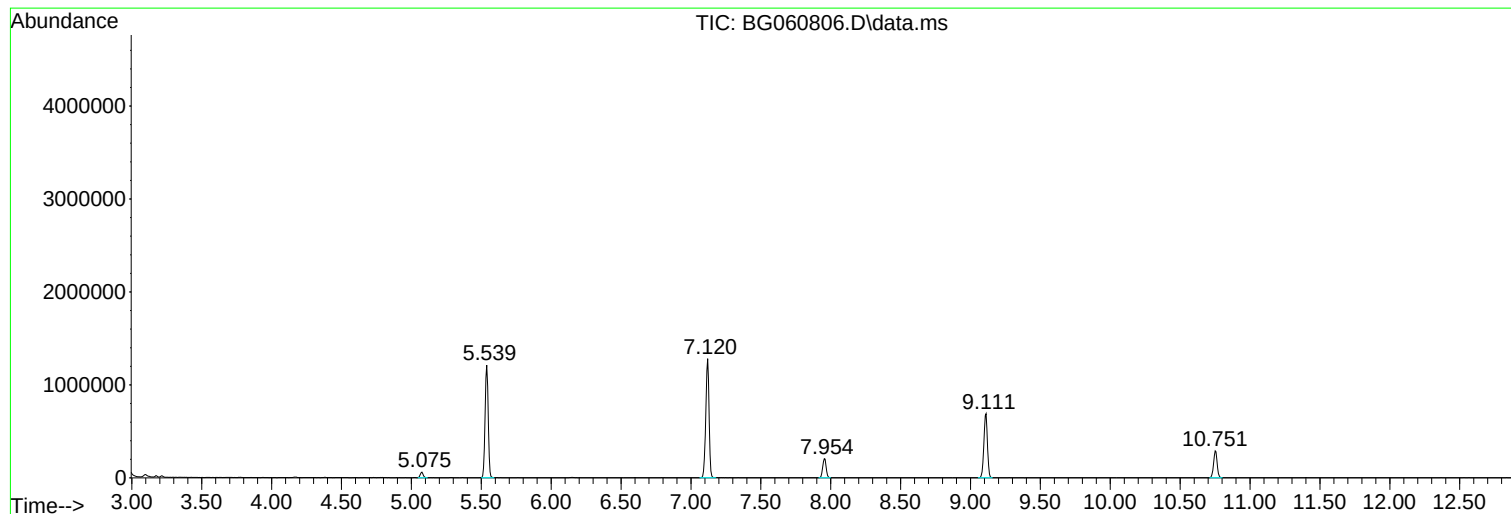
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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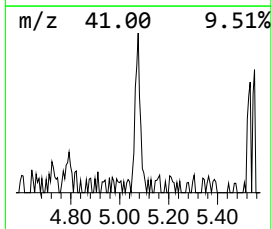
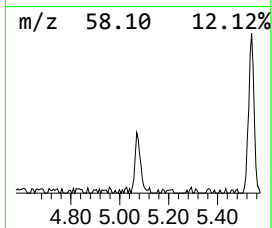
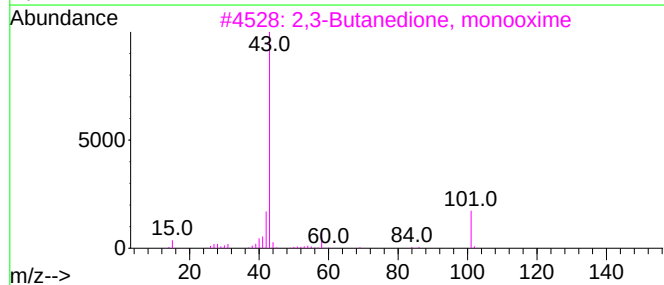
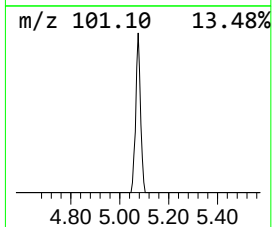
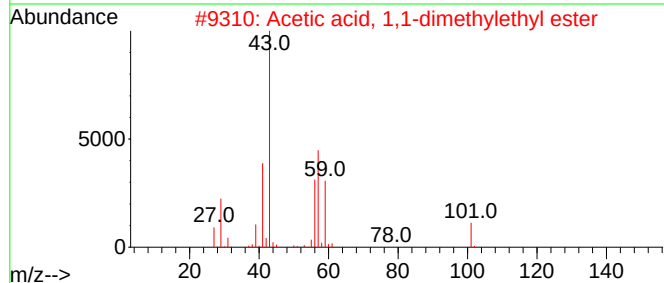
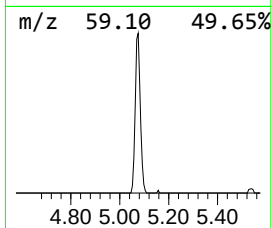
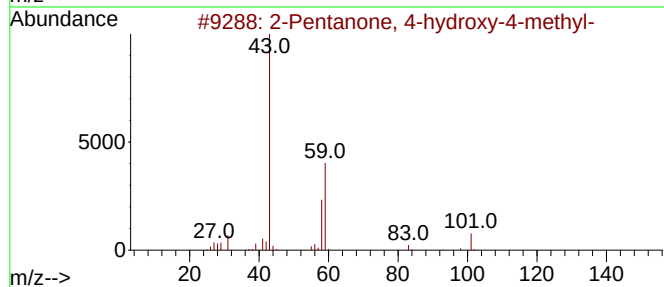
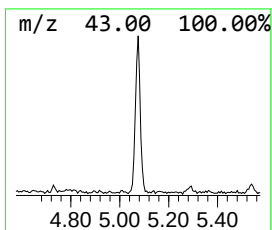
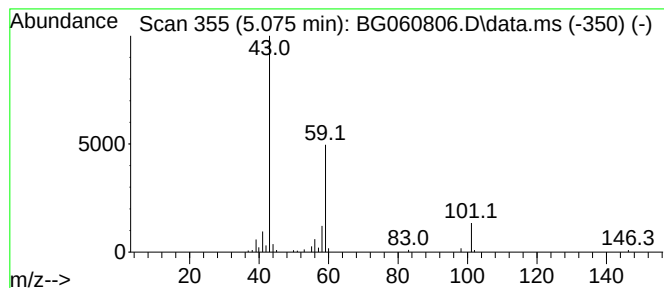
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	4.85 ng	84768	1,4-Dichlorobenzene-d4	7.960

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Propylamine	59	C3H9N	000107-10-8	9		
5	Butane	58	C4H10	000106-97-8	9		



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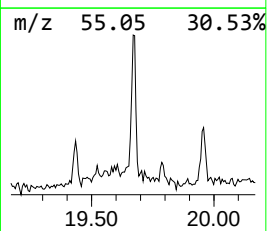
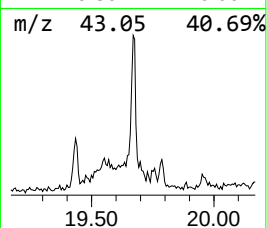
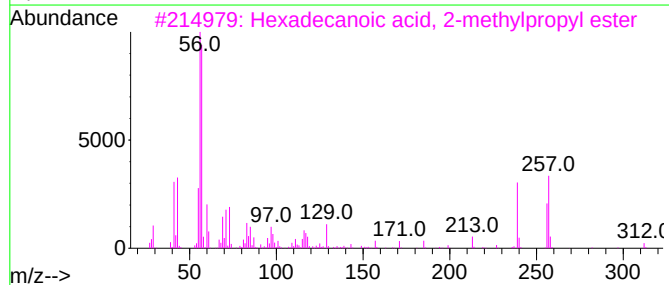
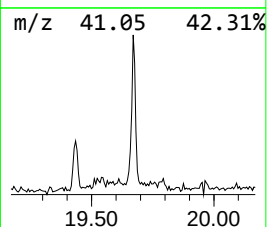
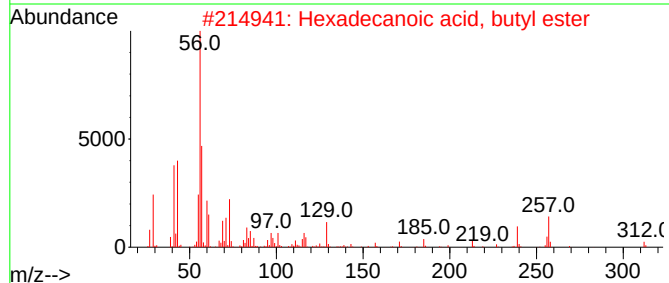
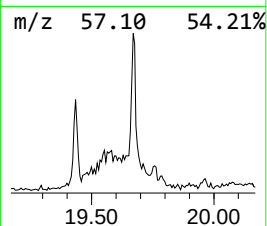
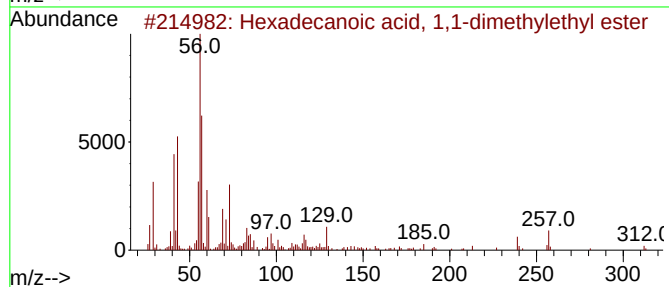
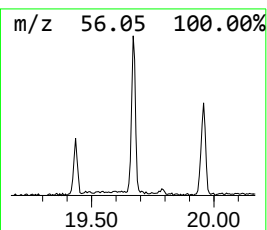
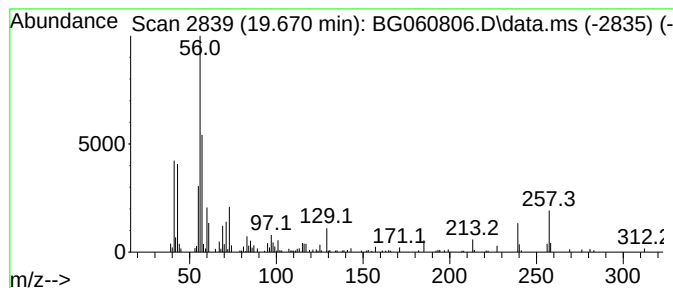
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.670	2.22 ng	163357	Chrysene-d12	21.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	93
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	89
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
5			Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38



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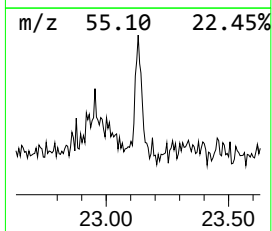
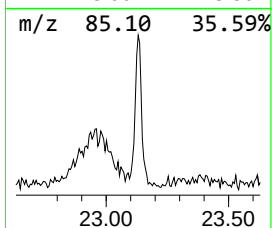
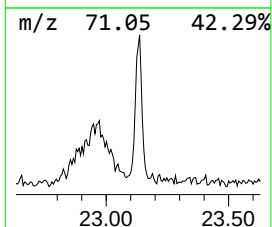
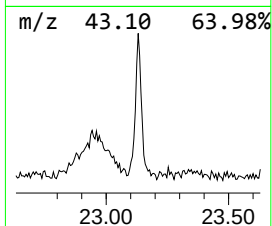
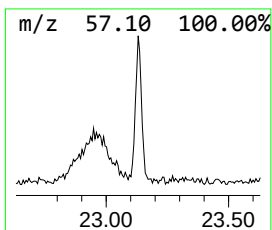
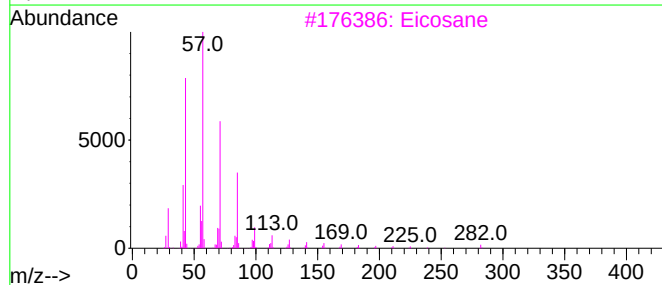
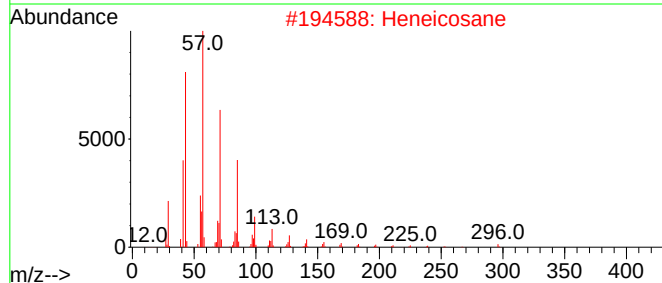
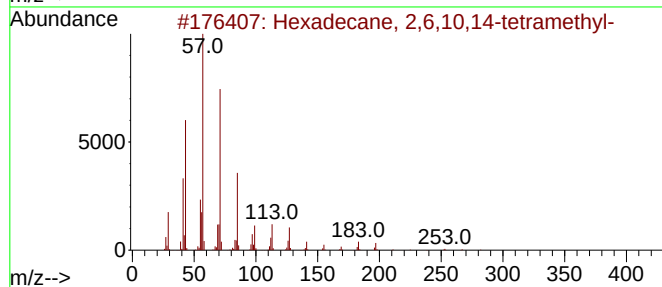
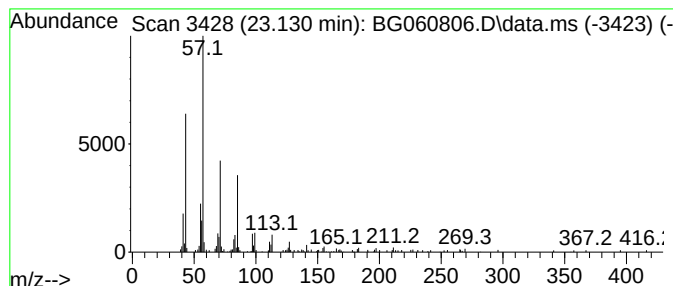
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Peak Number 3 Hexadecane, 2,6,10,14-tetra... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.130	2.20 ng	161403	Chrysene-d12	21.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	93		
2	Heneicosane	296	C21H44	000629-94-7	93		
3	Eicosane	282	C20H42	000112-95-8	87		
4	Tetracosane	338	C24H50	000646-31-1	83		
5	Hexacosane	366	C26H54	000630-01-3	81		



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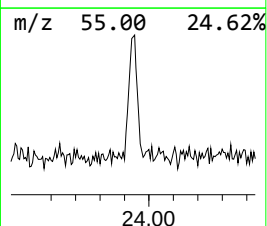
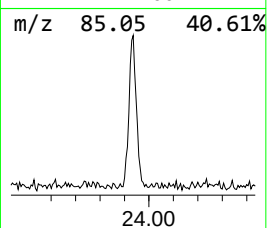
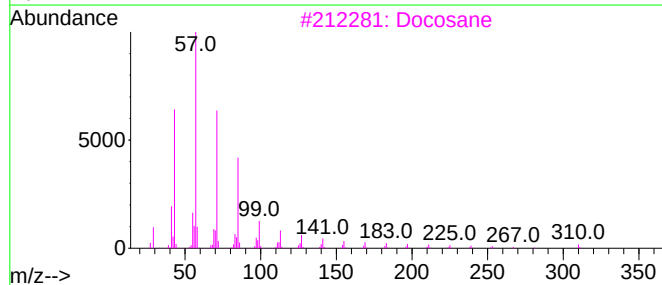
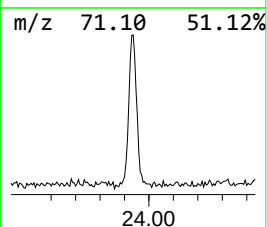
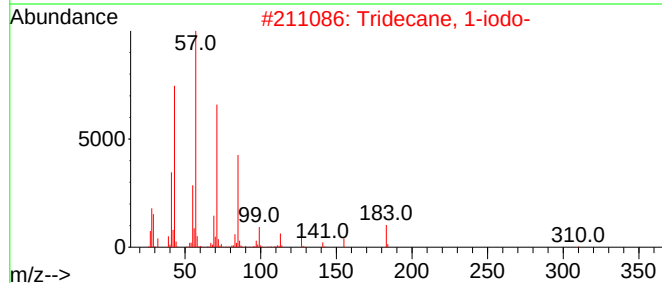
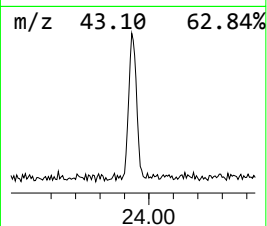
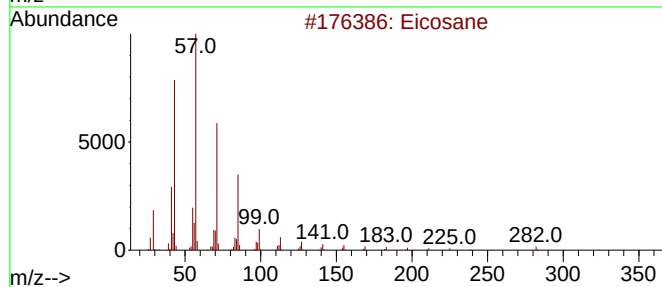
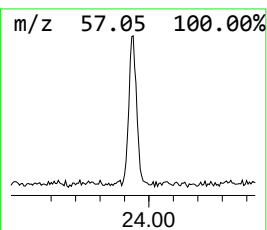
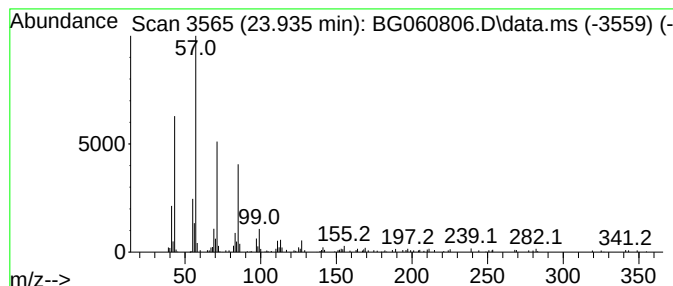
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Peak Number 4 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.935	2.90 ng	220045	Perylene-d12	24.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3			Docosane	310	C22H46	000629-97-0	87
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5			Triacontane	422	C30H62	000638-68-6	72



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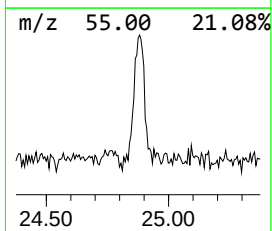
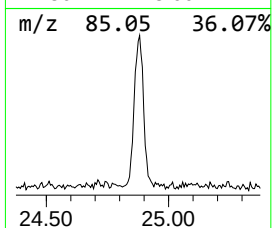
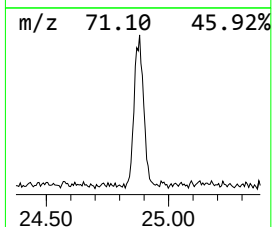
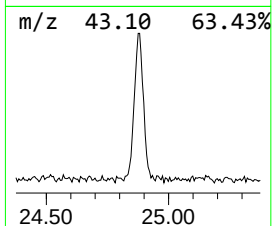
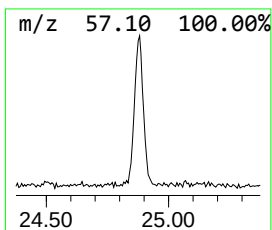
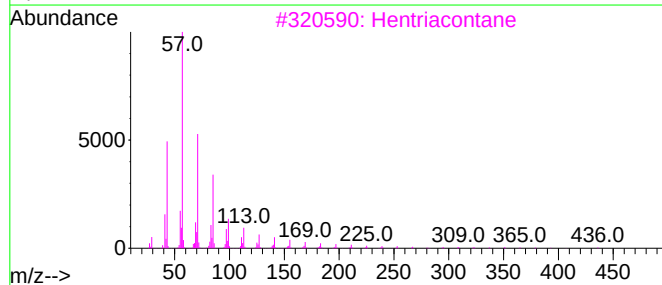
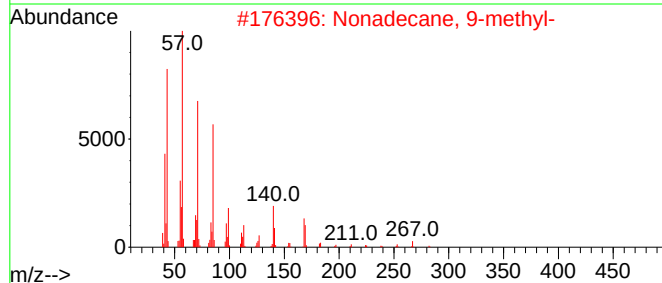
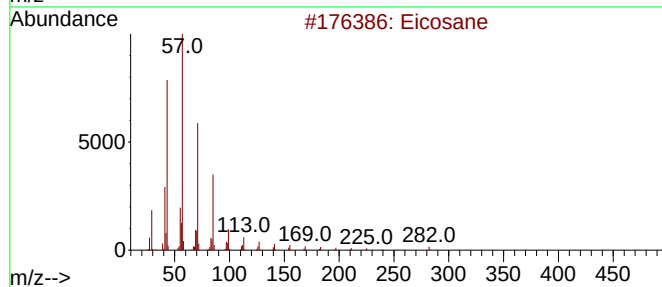
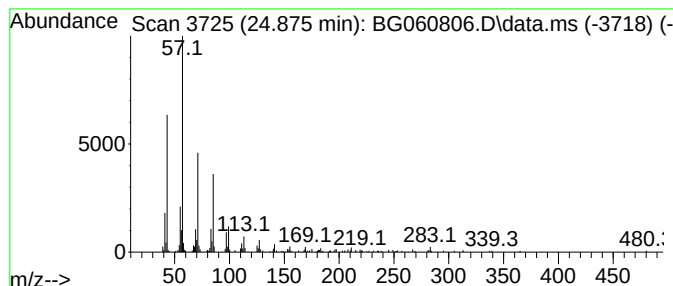
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Nonadecane, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.875	4.06 ng	307929	Perylene-d12	24.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Docosane	310	C22H46	000629-97-0	83
5			Hexacosane	366	C26H54	000630-01-3	83



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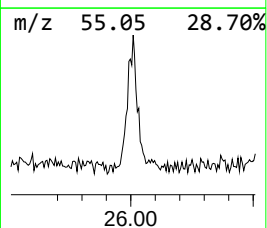
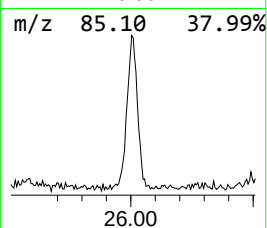
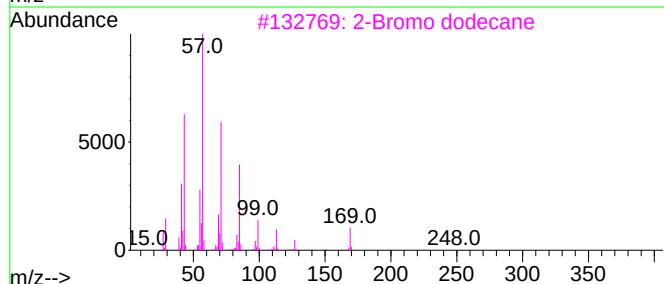
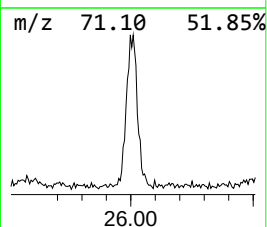
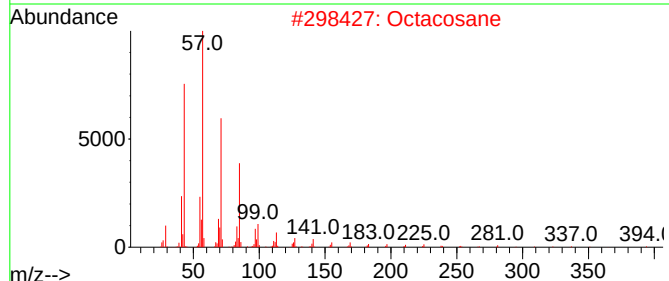
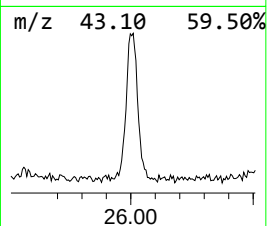
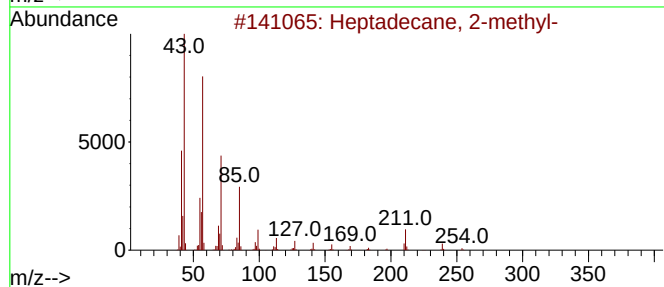
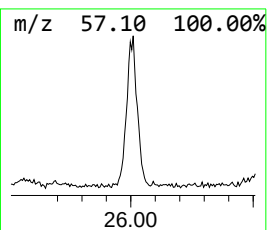
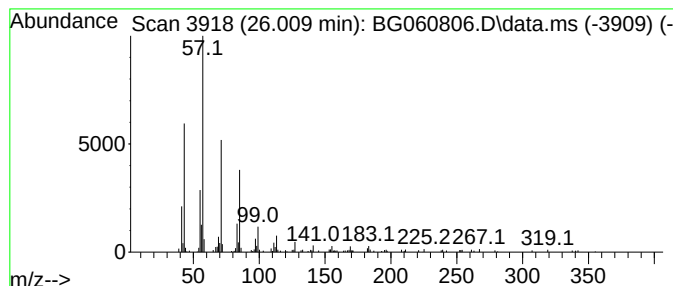
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.009	4.65 ng	352433	Perylene-d12	24.740

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 2-methyl-	254	C18H38	001560-89-0	83
2		Octacosane	394	C28H58	000630-02-4	83
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	80
4		Hentriacontane	437	C31H64	000630-04-6	80
5		Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
Data File : BG060806.D
Acq On : 6 Apr 2024 11:19
Operator : MA/JU
Sample : PB160028BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160028BL

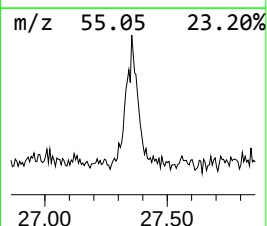
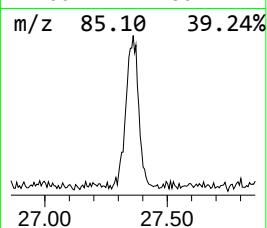
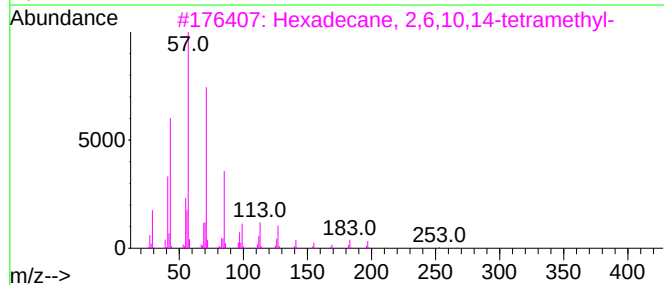
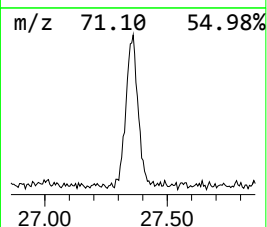
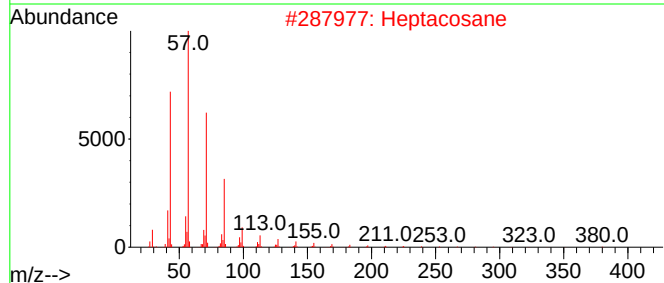
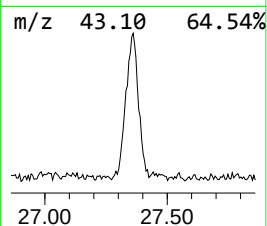
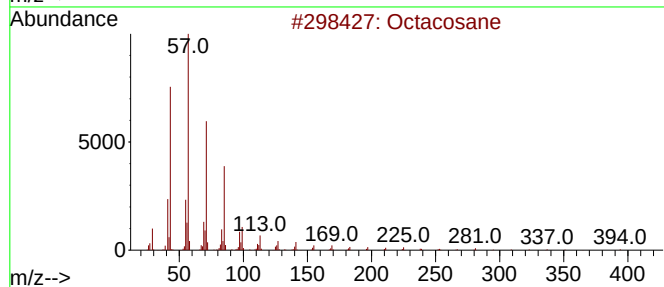
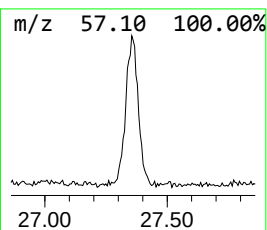
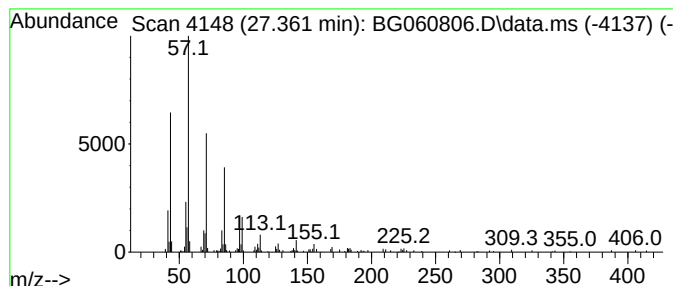
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.361	4.74 ng	358981	Perylene-d12	24.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Heptacosane	380	C27H56	000593-49-7	83
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	80
4			Docosane	310	C22H46	000629-97-0	72
5			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
Data File : BG060806.D
Acq On : 6 Apr 2024 11:19
Operator : MA/JU
Sample : PB160028BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160028BL

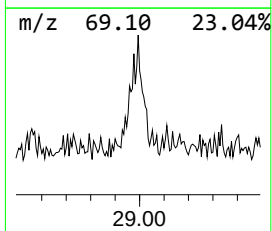
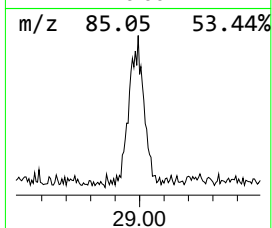
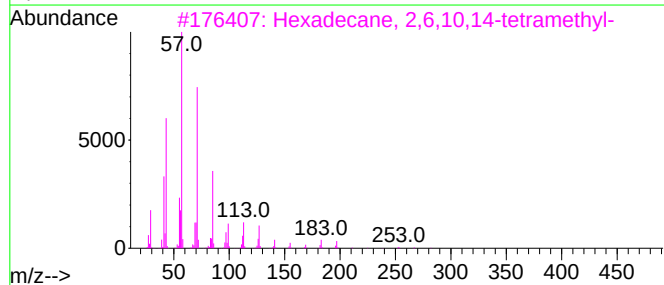
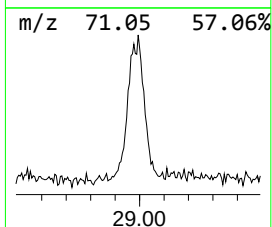
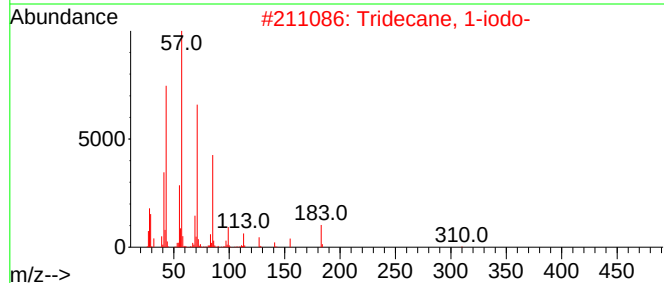
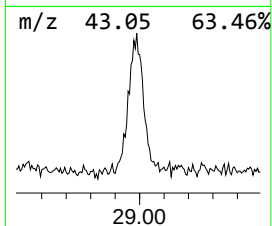
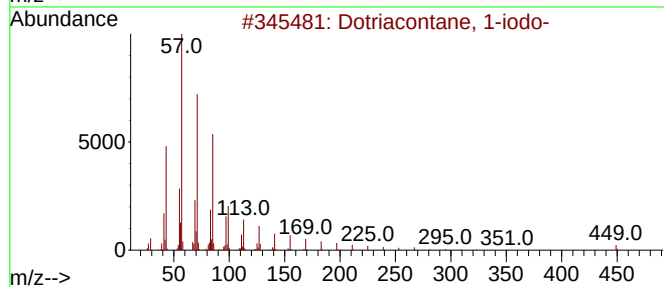
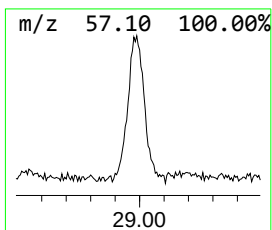
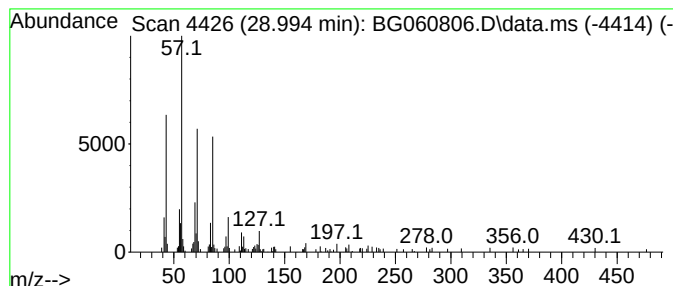
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dotriacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.994	3.75 ng	283874	Perylene-d12	24.740

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	78
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	72
3			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	58
4			Heptacosane	380	C27H56	000593-49-7	50
5			Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040624\
Data File : BG060806.D
Acq On : 6 Apr 2024 11:19
Operator : MA/JU
Sample : PB160028BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB160028BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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
2-Pentanone, 4-...	5.075	4.8	ng	84768	1	7.960	349769	20.0
Hexadecanoic ac...	19.670	2.2	ng	163357	5	21.597	1468860	20.0
Hexadecane, 2,6...	23.130	2.2	ng	161403	5	21.597	1468860	20.0
Eicosane	23.935	2.9	ng	220045	6	24.740	1515700	20.0
Nonadecane, 9-m...	24.875	4.1	ng	307929	6	24.740	1515700	20.0
Heptadecane, 2-...	26.009	4.7	ng	352433	6	24.740	1515700	20.0
Octacosane	27.361	4.7	ng	358981	6	24.740	1515700	20.0
Dotriacontane, ...	28.994	3.8	ng	283874	6	24.740	1515700	20.0