

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
 Data File : BM039950.D
 Acq On : 18 May 2023 15:46
 Operator : CG/JU
 Sample : 02828-05
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-5

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_M\Methods\8270-BM051223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039950.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.125	10	15	20	rBV	2544958	2669292	8.56%	1.873%
2	5.096	343	350	360	rBV	1525734	2078387	6.67%	1.458%
3	5.566	419	430	443	rBV	9430182	13081869	41.96%	9.180%
4	7.172	695	703	717	rBV	8449463	13075576	41.94%	9.175%
5	8.019	840	847	855	rBV	1721599	2685329	8.61%	1.884%
6	9.189	1037	1046	1055	rBV	5073482	7966293	25.55%	5.590%
7	10.836	1318	1326	1334	rBV	2291818	3749278	12.03%	2.631%
8	13.289	1735	1743	1754	rBV	14458744	19384924	62.18%	13.603%
9	14.654	1969	1975	1984	rBV	2999555	4434197	14.22%	3.112%
10	16.012	2200	2206	2212	rBV	466024	657309	2.11%	0.461%
11	16.142	2221	2228	2245	rBV	11293104	15440142	49.53%	10.834%
12	17.401	2436	2442	2450	rBV	3624645	4963507	15.92%	3.483%
13	18.295	2588	2594	2604	rBV	2214863	3556287	11.41%	2.495%
14	19.571	2805	2811	2831	rBV	1013643	1981182	6.35%	1.390%
15	19.824	2849	2854	2866	rVB	414248	590608	1.89%	0.414%
16	20.018	2881	2887	2892	rBV	29236821	31176070	100.00%	21.876%
17	21.283	3098	3102	3114	rBV	761171	1049916	3.37%	0.737%
18	21.577	3146	3152	3165	rBV	3937919	5272152	16.91%	3.700%
19	22.871	3367	3372	3381	rVB	2494053	3427948	11.00%	2.405%
20	24.030	3562	3569	3584	rVB	2789905	5269319	16.90%	3.698%

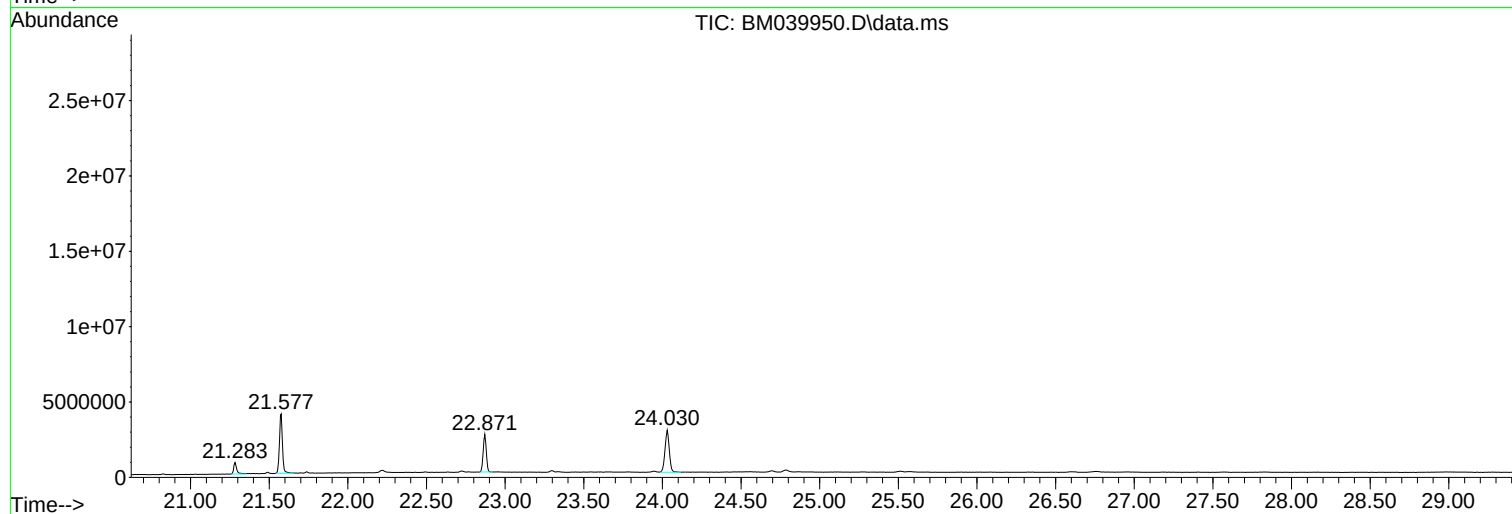
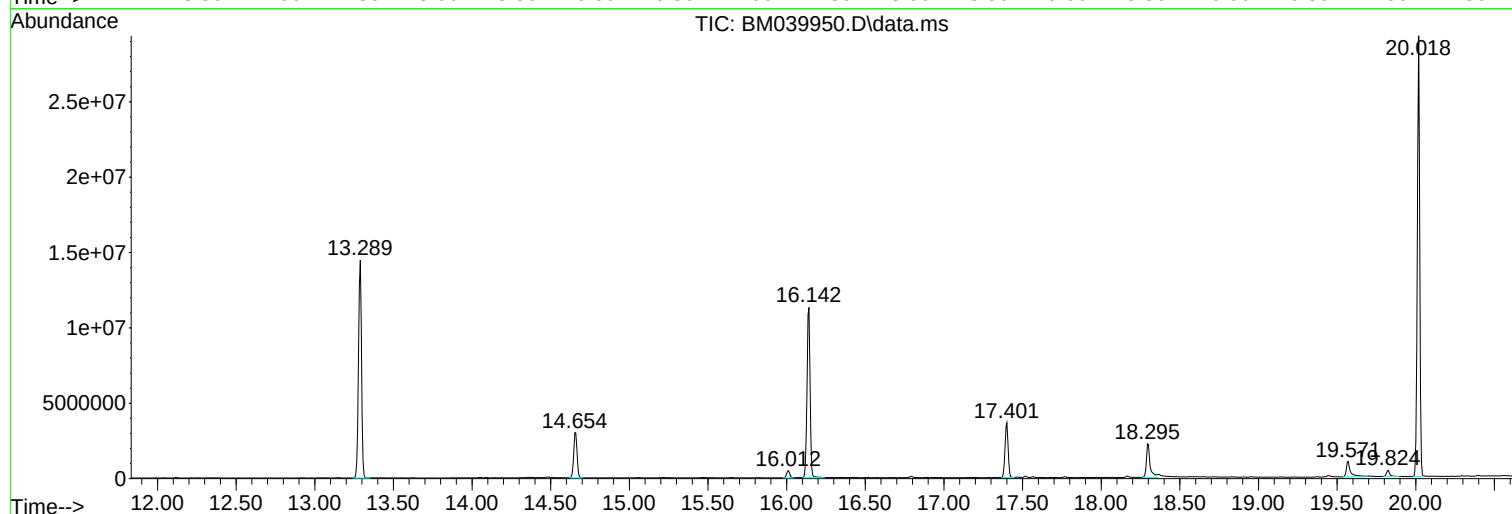
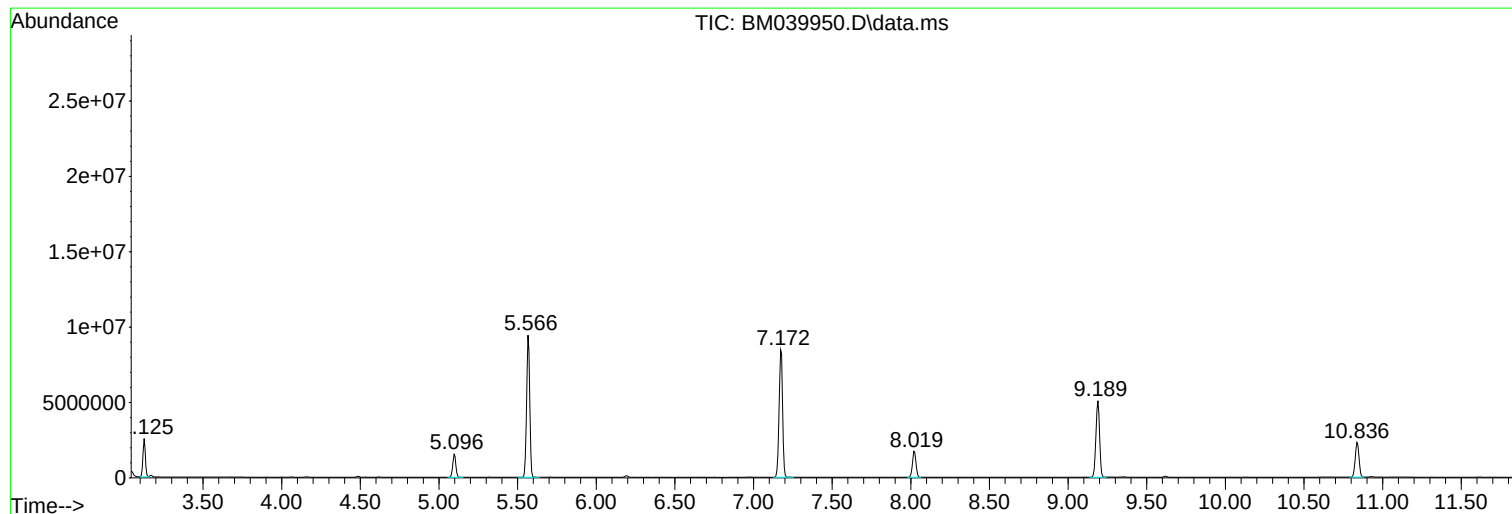
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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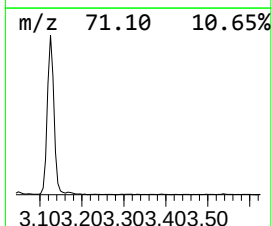
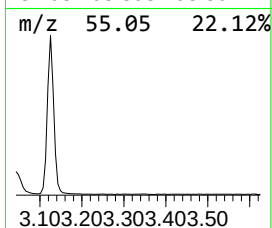
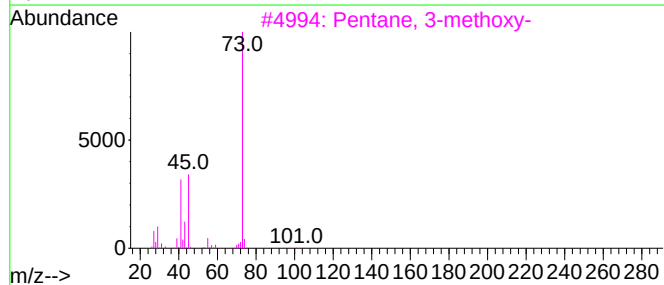
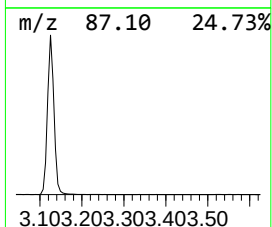
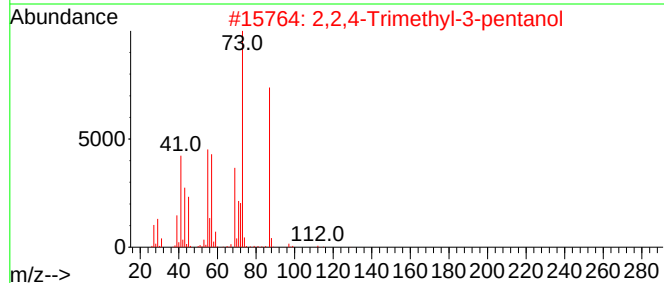
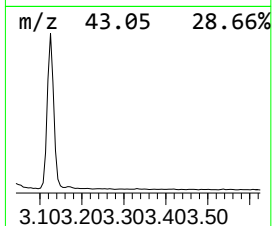
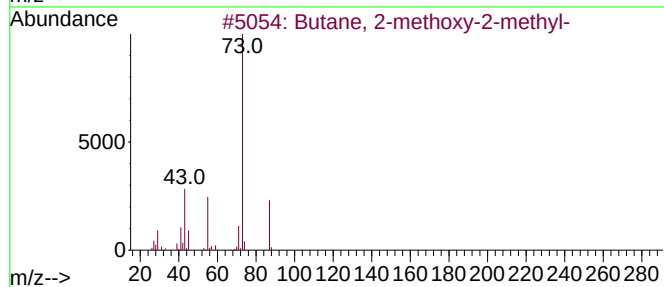
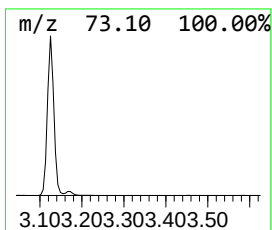
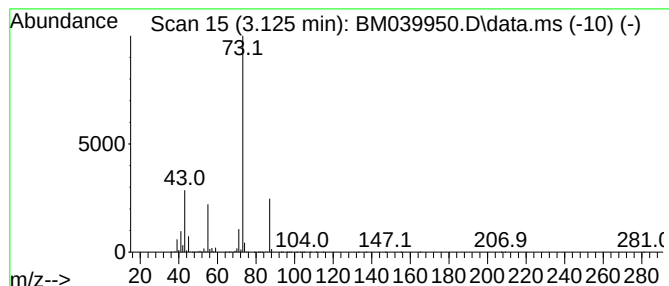
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.125	19.88 ng	2669290	1,4-Dichlorobenzene-d4	8.025

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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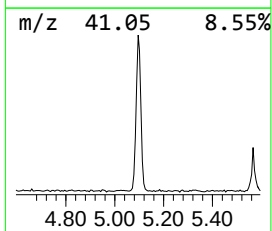
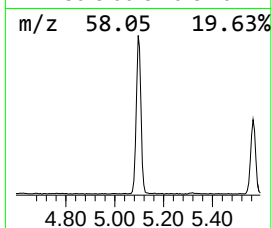
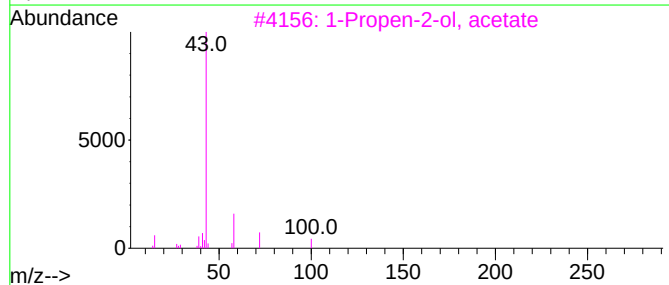
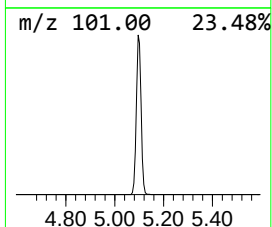
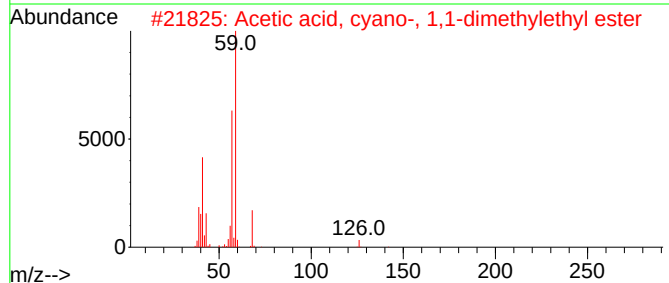
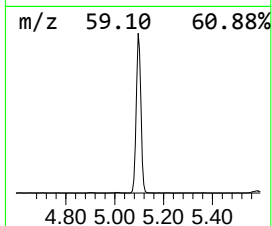
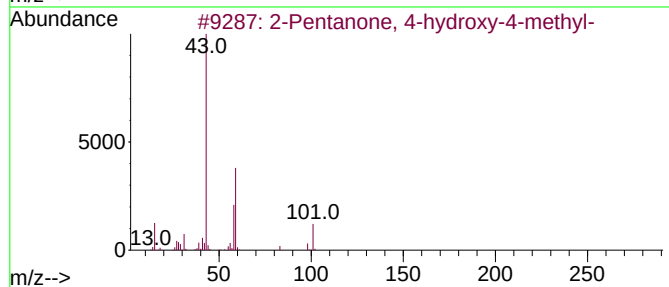
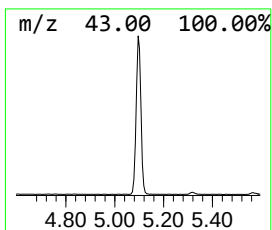
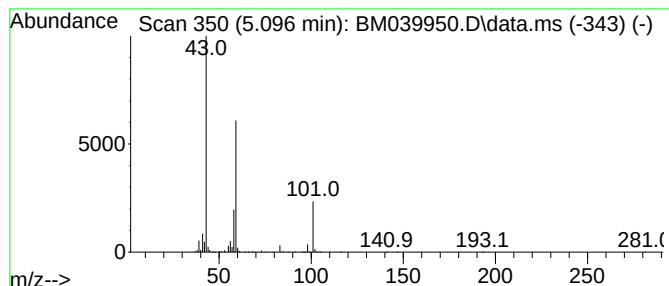
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.096	15.48 ng	2078390	1,4-Dichlorobenzene-d4	8.025	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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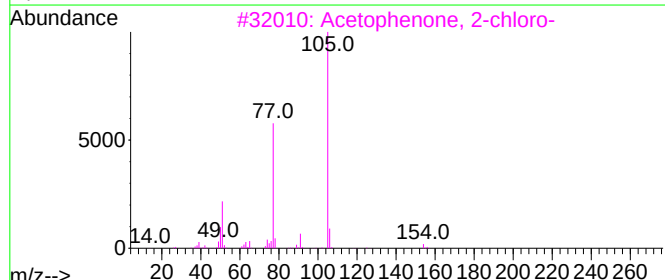
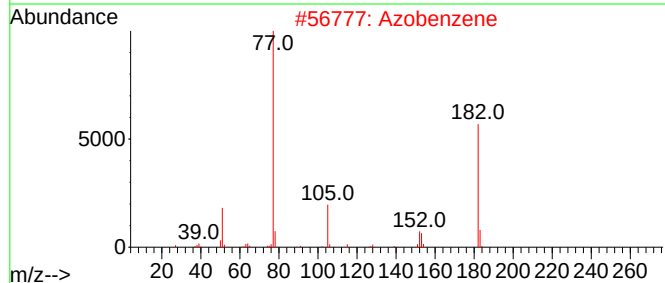
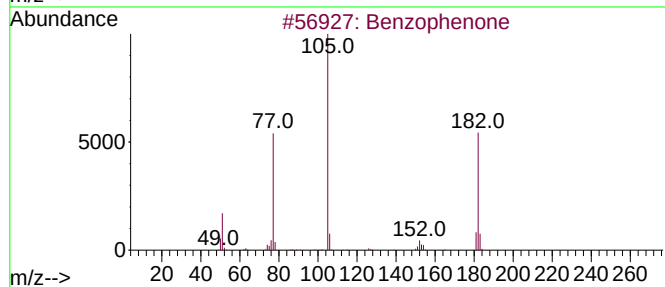
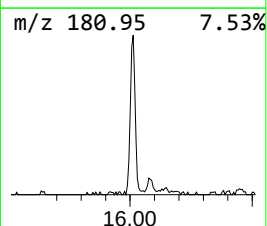
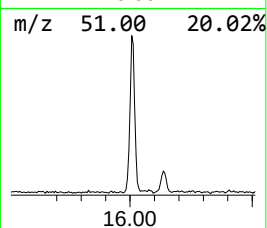
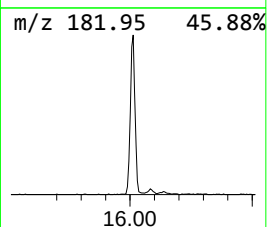
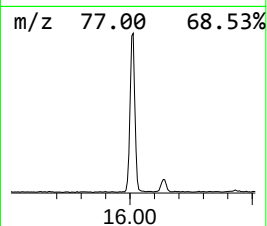
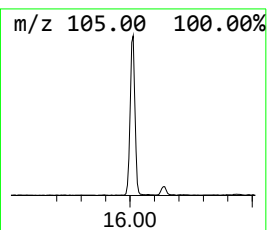
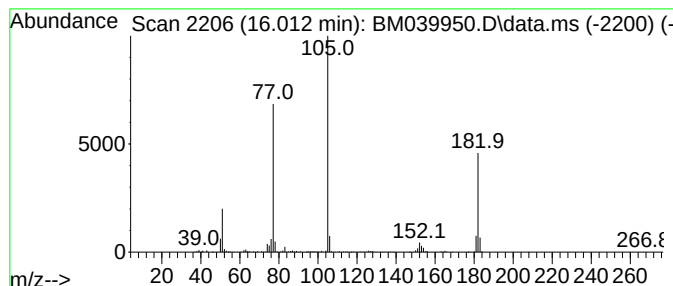
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.012	2.96 ng	657309	Acenaphthene-d10	14.660

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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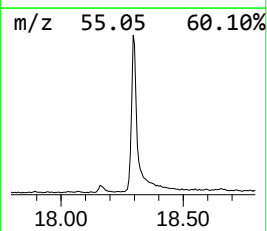
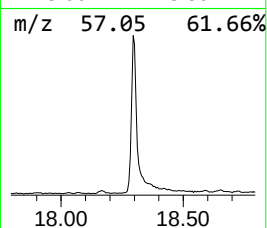
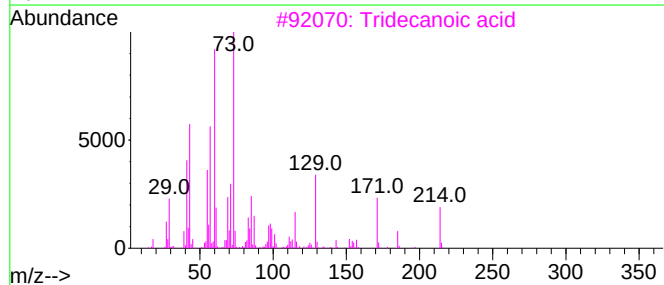
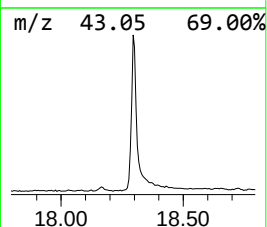
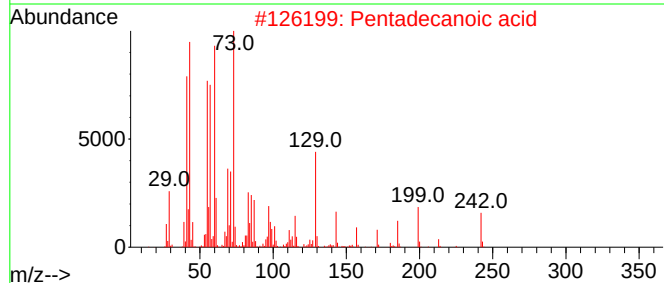
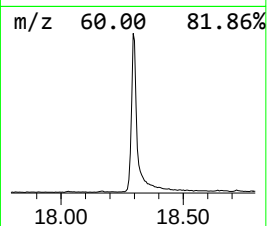
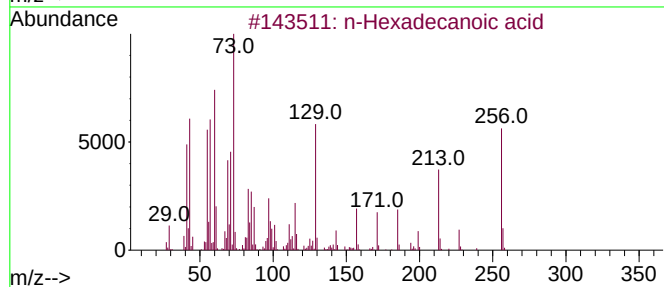
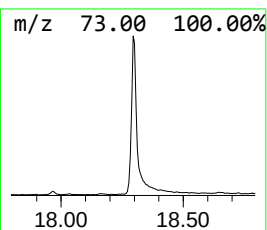
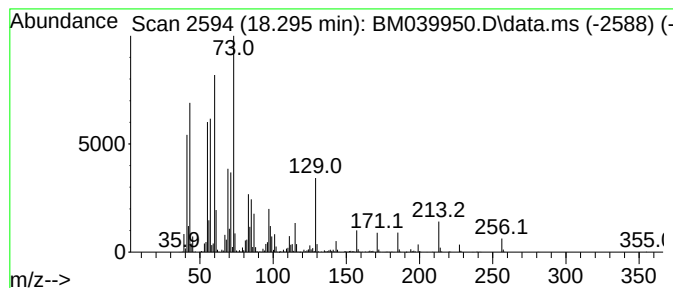
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.295	14.33 ng	3556290	Phenanthrene-d10	17.401

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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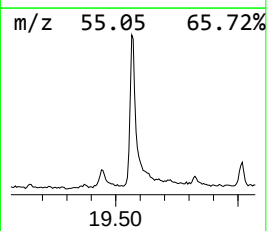
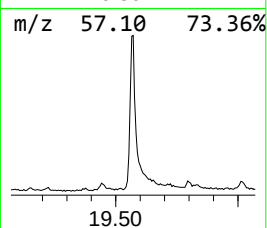
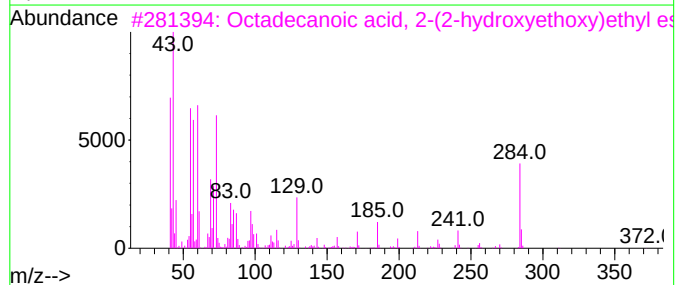
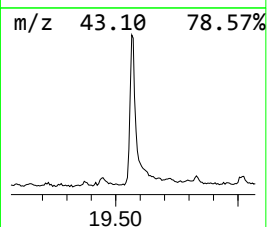
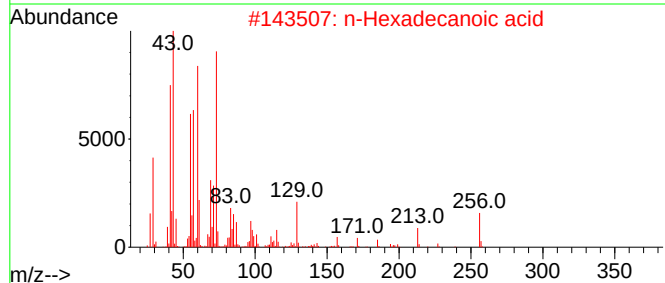
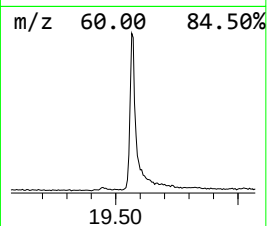
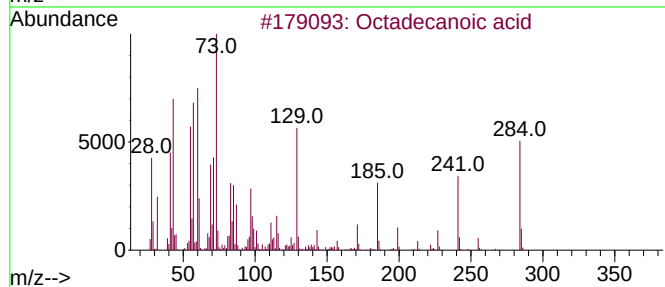
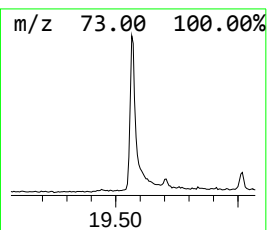
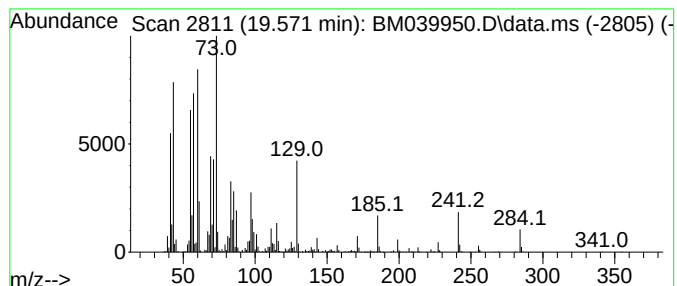
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.571	7.52 ng	1981180	Chrysene-d12	21.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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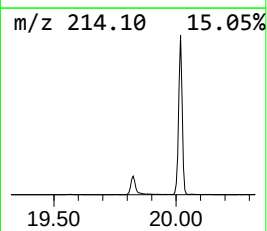
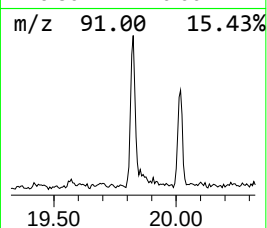
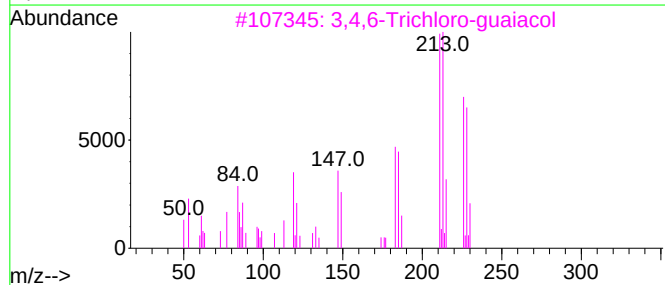
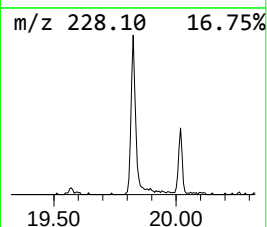
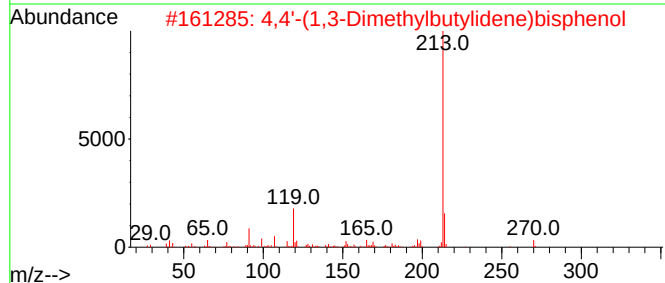
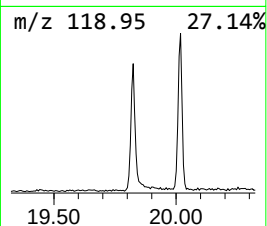
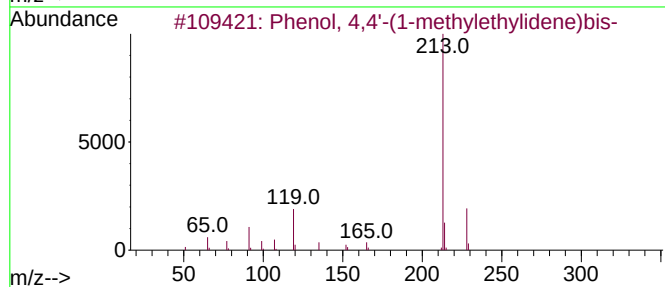
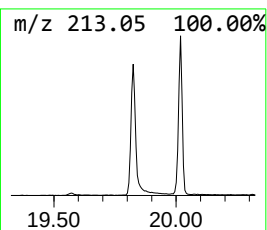
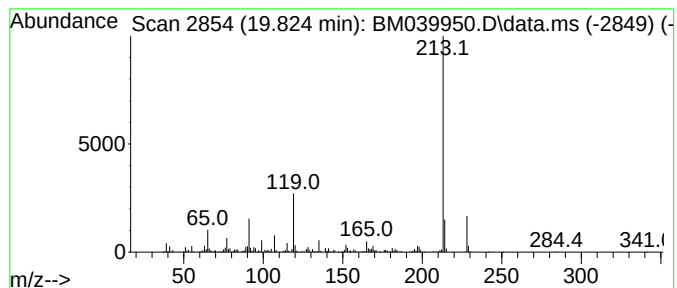
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.824	2.24 ng	590608	Chrysene-d12	21.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene)bis...	228	C15H16O2	000080-05-7	98
2			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	72
3			3,4,6-Trichloro-guaiacol	226	C7H5Cl3O2	060712-44-9	59
4			Diphenolic acid	286	C17H18O4	000126-00-1	56
5			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
Data File : BM039950.D
Acq On : 18 May 2023 15:46
Operator : CG/JU
Sample : 02828-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-5

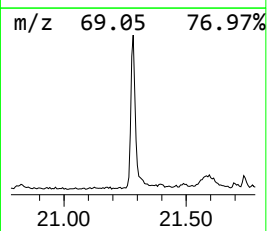
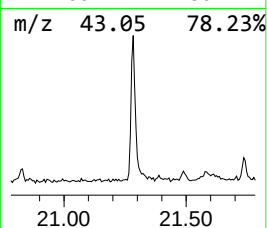
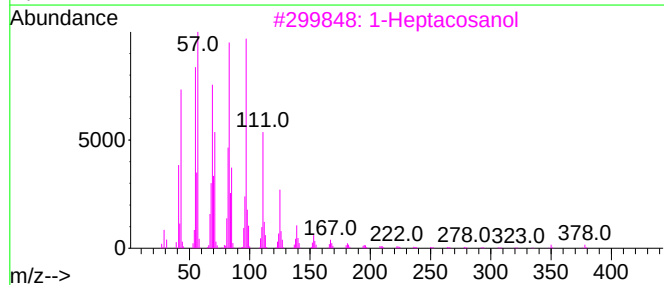
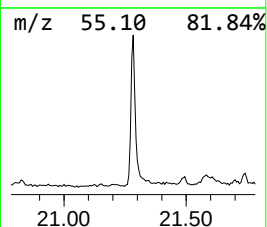
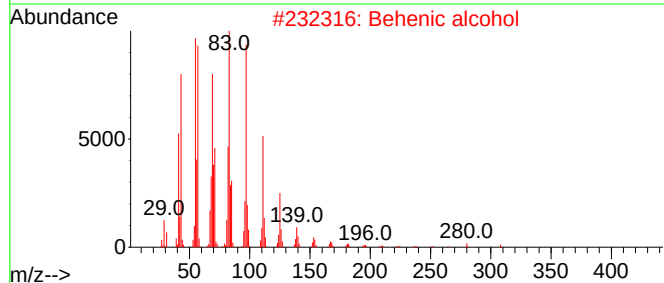
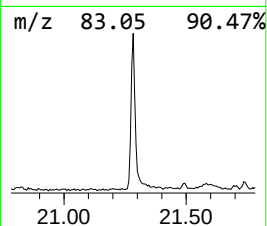
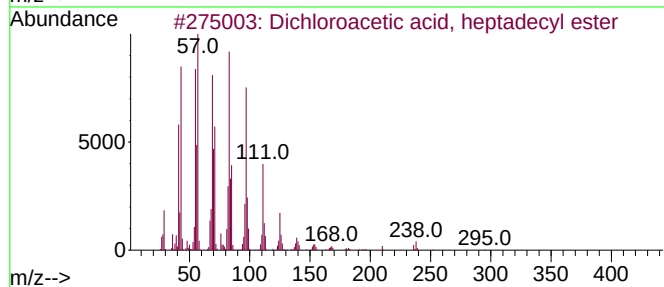
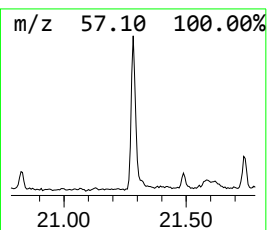
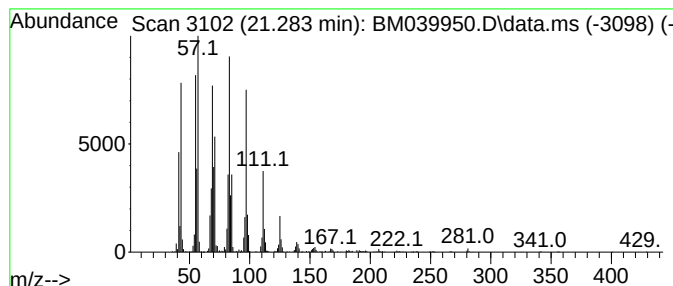
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.283	3.98 ng	1049920	Chrysene-d12	21.577

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Behenic alcohol	326	C22H46O	000661-19-8	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
Data File : BM039950.D
Acq On : 18 May 2023 15:46
Operator : CG/JU
Sample : 02828-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-5

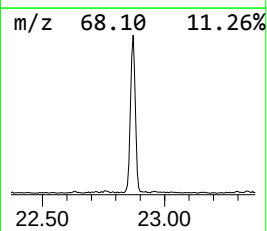
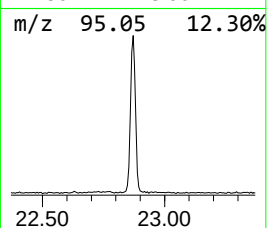
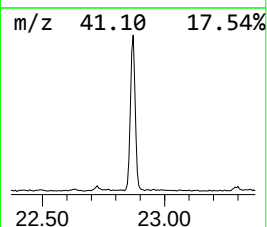
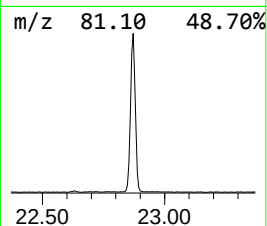
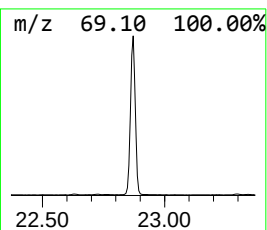
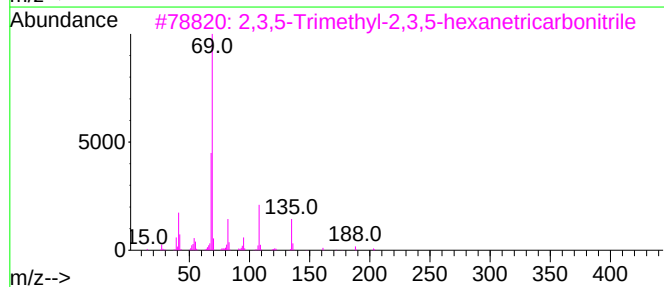
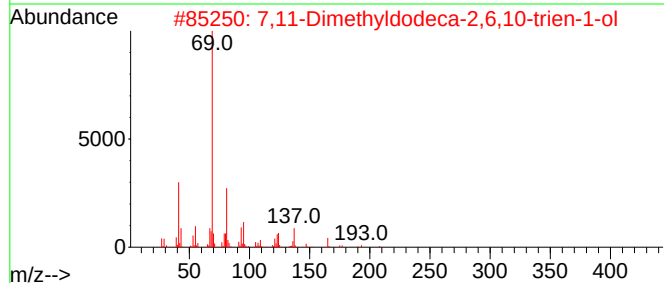
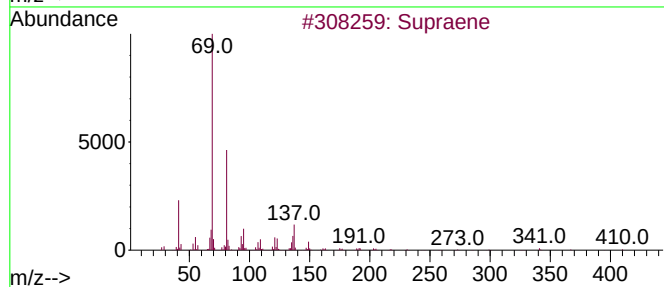
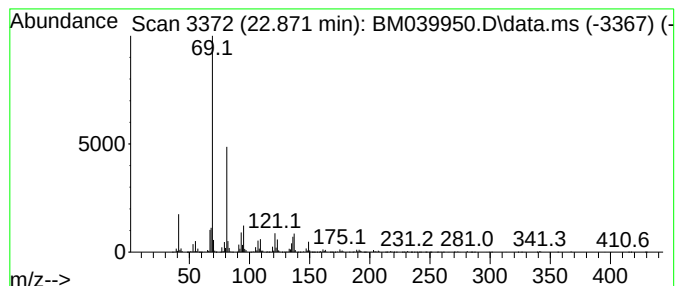
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.871	13.01 ng	3427950	Perylene-d12	24.030

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59
4			3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	59
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051823\
Data File : BM039950.D
Acq On : 18 May 2023 15:46
Operator : CG/JU
Sample : 02828-05
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM051223.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
Butane, 2-metho...	3.125	19.9	ng	2669290	1	8.025	2685330	20.0
2-Pentanone, 4-...	5.096	15.5	ng	2078390	1	8.025	2685330	20.0
Benzophenone	16.012	3.0	ng	657309	3	14.660	4434200	20.0
n-Hexadecanoic ...	18.295	14.3	ng	3556290	4	17.401	4963510	20.0
Octadecanoic acid	19.571	7.5	ng	1981180	5	21.577	5272150	20.0
Phenol, 4,4'-(1...	19.824	2.2	ng	590608	5	21.577	5272150	20.0
Dichloroacetic ...	21.283	4.0	ng	1049920	5	21.577	5272150	20.0
Supraene	22.871	13.0	ng	3427950	6	24.030	5269320	20.0