

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
 Data File : BM044744.D
 Acq On : 22 Mar 2024 20:52
 Operator : MA/JU
 Sample : P1788-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PEZOMETER-200

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-BM031324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	298	304	319	rVB	340381	564695	7.16%	1.343%
2	5.310	371	378	392	rBV	1027263	1718051	21.79%	4.087%
3	6.869	635	643	654	rBV	580520	1003213	12.72%	2.387%
4	7.687	775	782	789	rBV	765165	1237335	15.69%	2.943%
5	8.775	959	967	972	rBV	60314	100154	1.27%	0.238%
6	8.851	972	980	991	rBV	2300849	3900167	49.47%	9.278%
7	9.040	993	1012	1019	rVV	755418	2481116	31.47%	5.902%
8	9.292	1050	1055	1061	rVV	53792	84982	1.08%	0.202%
9	9.351	1061	1065	1073	rVB	80035	129712	1.65%	0.309%
10	9.857	1147	1151	1158	rVB2	60700	113169	1.44%	0.269%
11	10.257	1212	1219	1229	rBV2	102466	212153	2.69%	0.505%
12	10.463	1242	1254	1269	rBV	938171	1659779	21.05%	3.948%
13	12.945	1669	1676	1689	rBV	5064773	7585551	96.21%	18.045%
14	13.551	1769	1779	1785	rBV	106136	188847	2.40%	0.449%
15	14.327	1904	1911	1922	rBV	1197739	1782862	22.61%	4.241%
16	14.986	2016	2023	2032	rBV	489463	716082	9.08%	1.703%
17	15.298	2070	2076	2085	rBV	104091	201761	2.56%	0.480%
18	15.827	2159	2166	2180	rBV	2272386	3394128	43.05%	8.074%
19	15.951	2182	2187	2193	rBV	61433	107849	1.37%	0.257%
20	17.080	2373	2379	2390	rBV	1246535	1838090	23.31%	4.373%
21	17.992	2529	2534	2545	rBV	343577	549477	6.97%	1.307%
22	19.286	2749	2754	2763	rBV	224979	369252	4.68%	0.878%
23	19.427	2775	2778	2783	rVB	77547	87060	1.10%	0.207%
24	19.545	2795	2798	2805	rVB	74615	100676	1.28%	0.239%
25	19.727	2823	2829	2838	rBV	6183237	7883966	100.00%	18.755%
26	21.015	3045	3048	3053	rVB	102386	122444	1.55%	0.291%
27	21.280	3088	3093	3099	rBV	1503672	1919795	24.35%	4.567%
28	23.521	3468	3474	3485	rVB	1016195	1983948	25.16%	4.720%

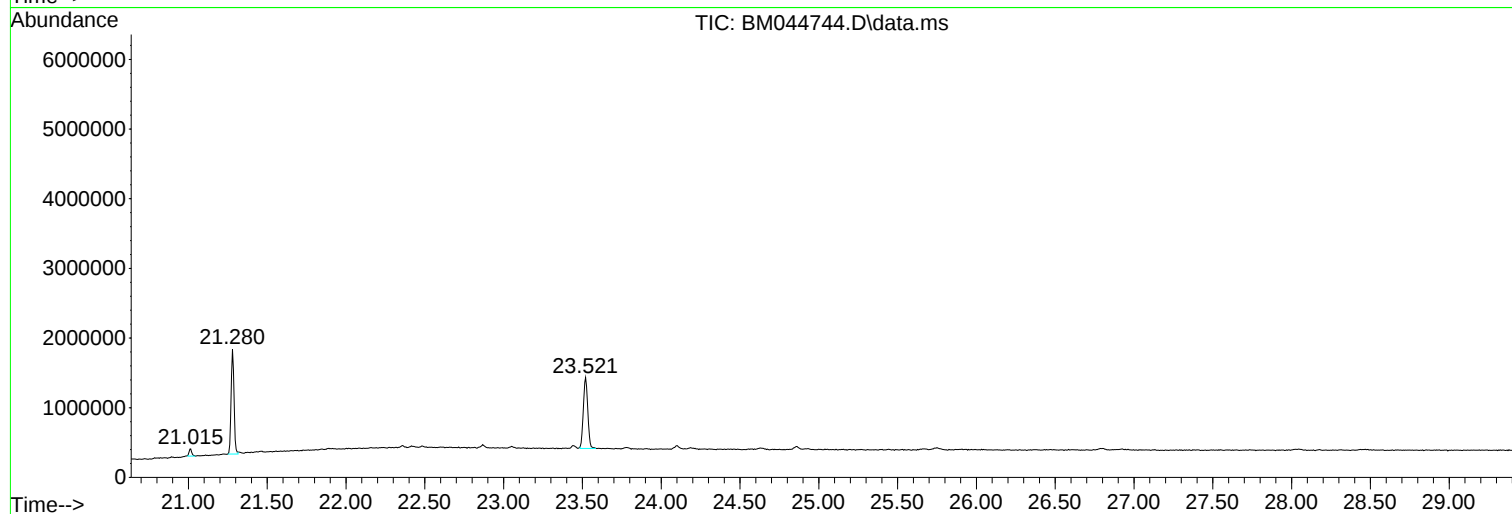
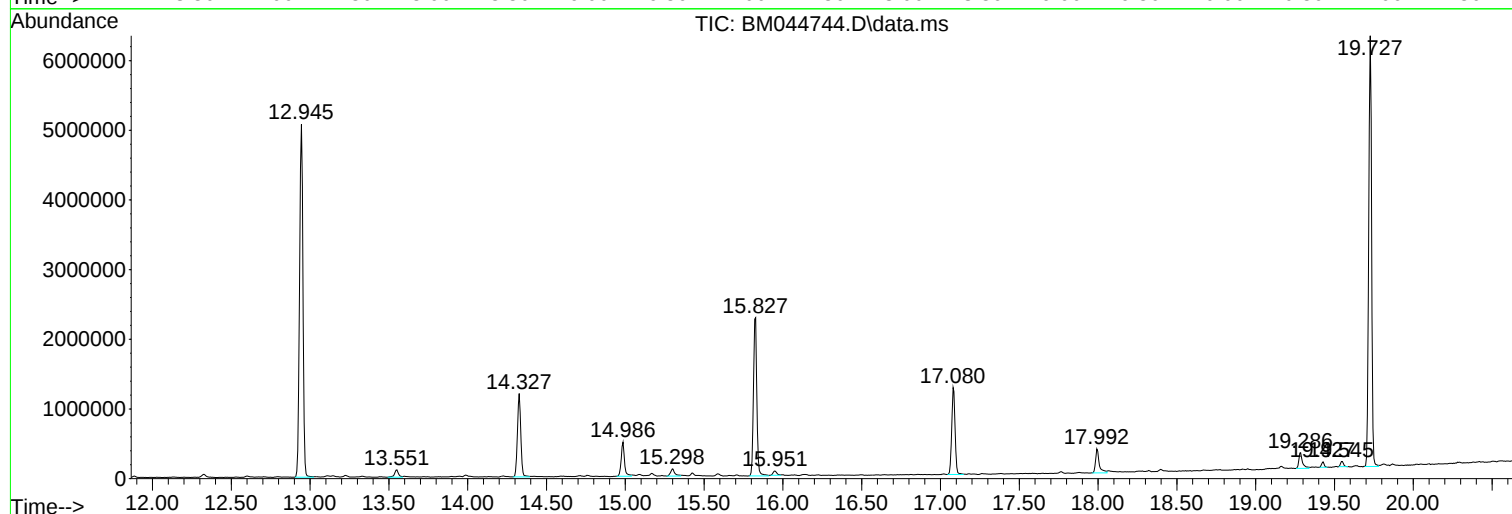
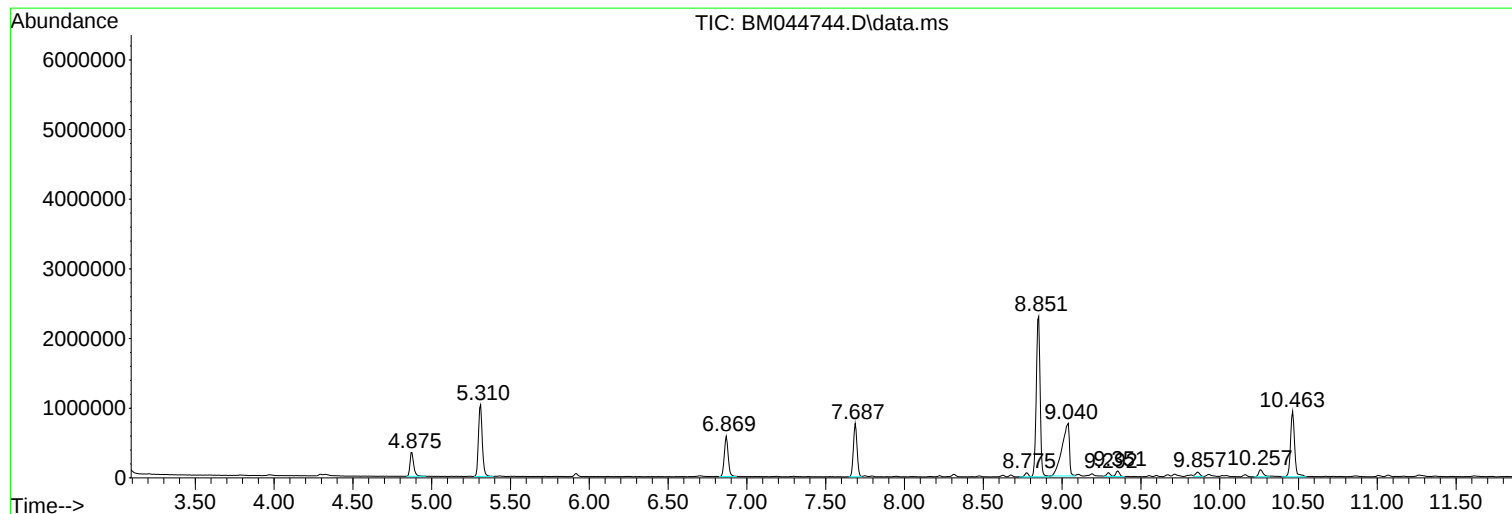
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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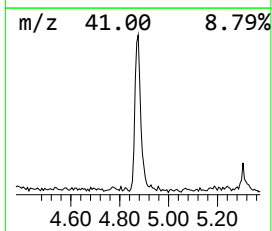
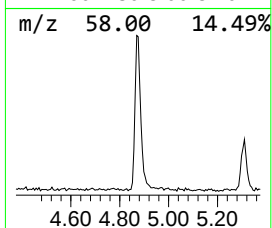
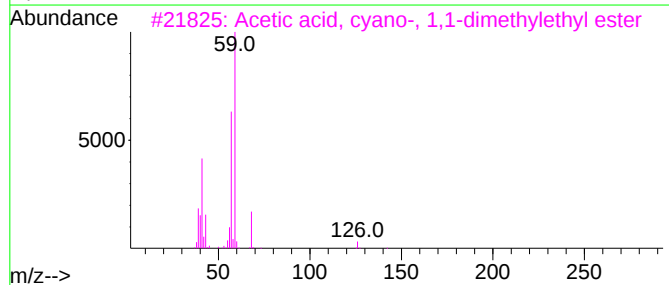
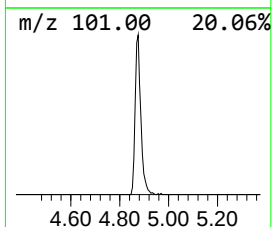
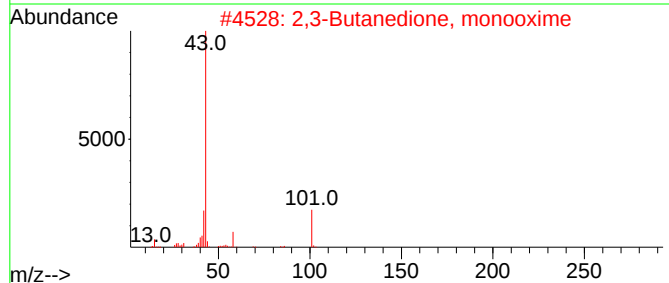
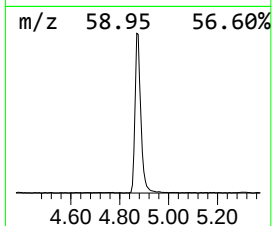
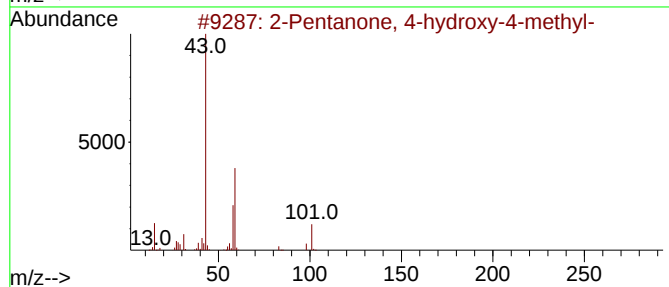
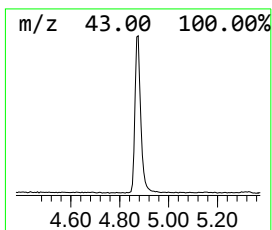
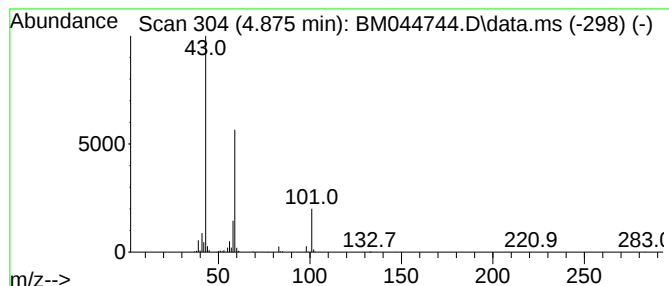
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	9.13 ng	564695	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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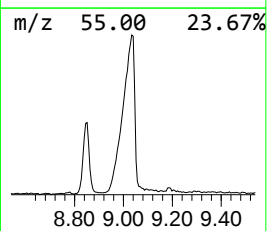
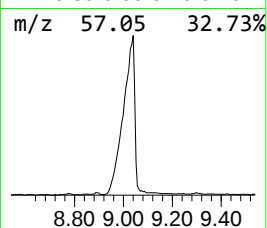
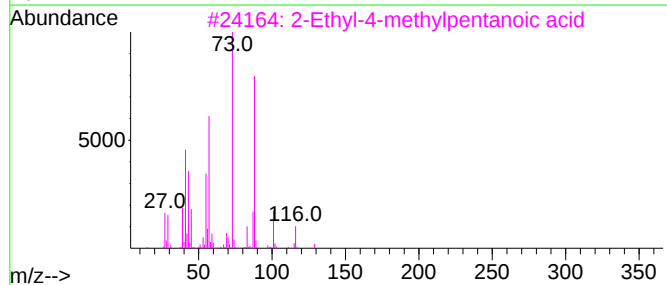
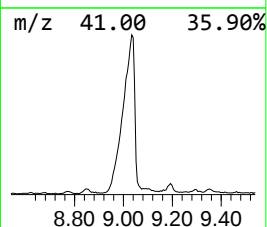
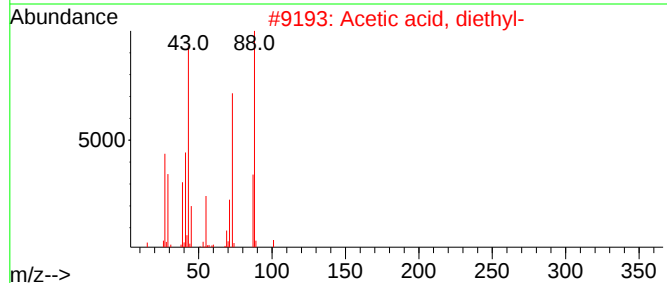
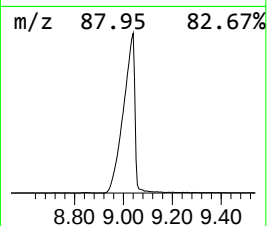
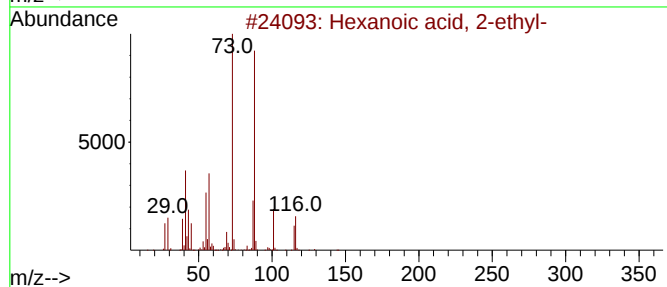
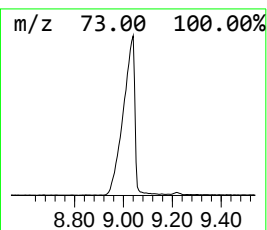
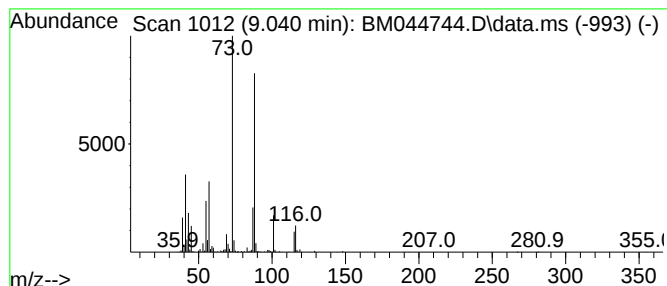
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Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.040	40.10 ng	2481120	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	59
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	56
4			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
5			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	53



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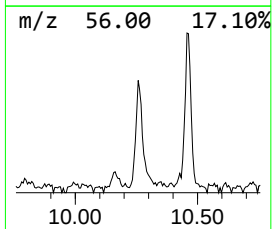
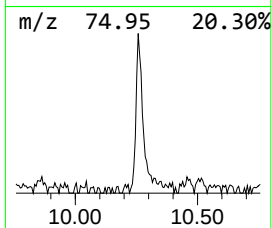
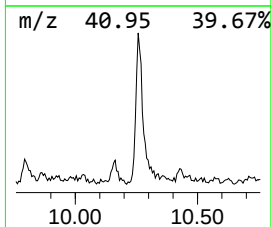
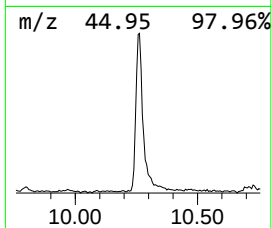
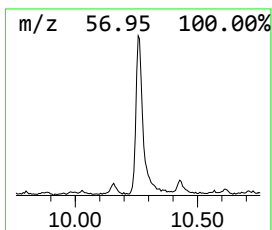
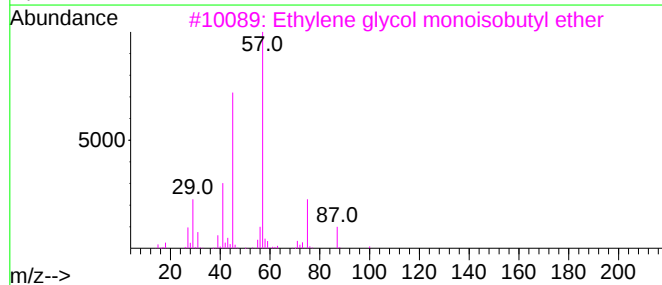
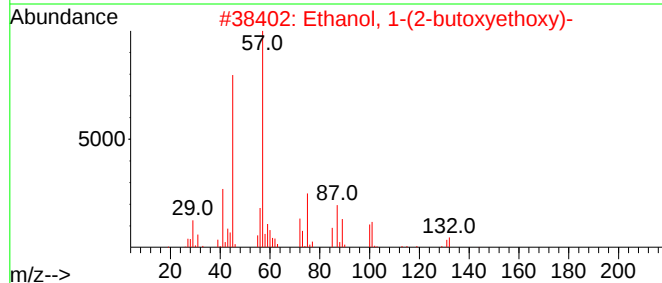
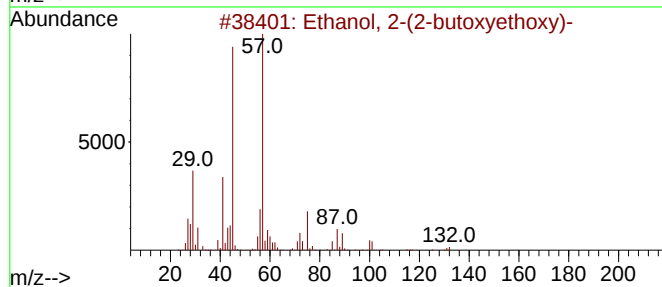
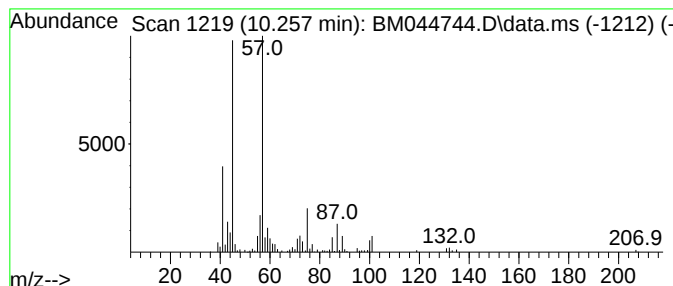
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.257	2.56 ng	212153	Naphthalene-d8	10.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	72
4			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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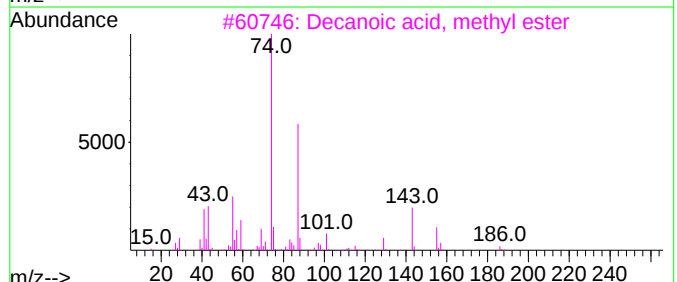
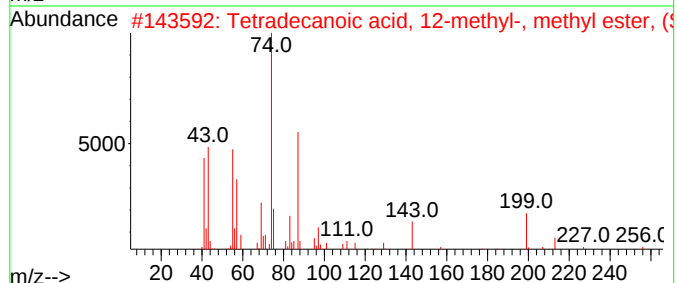
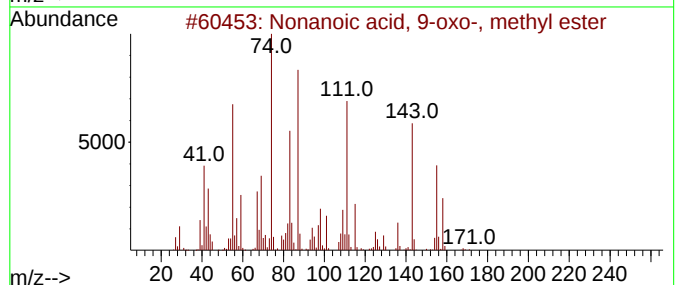
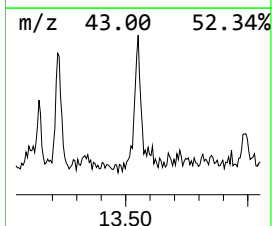
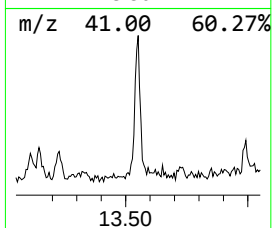
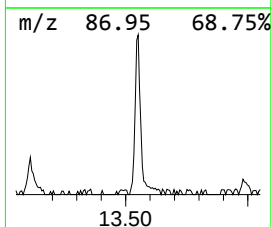
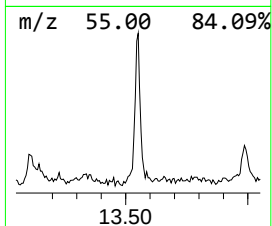
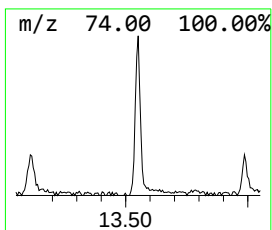
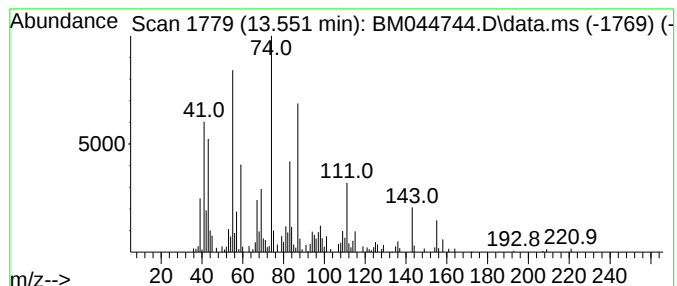
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Peak Number 4 Nonanoic acid, 9-oxo-, meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.551	2.12 ng	188847	Acenaphthene-d10	14.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	90
2			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	062691-05-8	47
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	43
4			Cyclopentaneundecanoic acid, met...	268	C17H32O2	025779-85-5	38
5			Undecanoic acid, methyl ester	200	C12H24O2	001731-86-8	38



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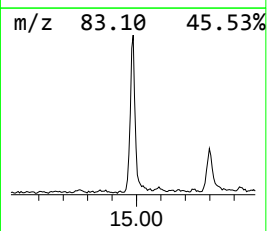
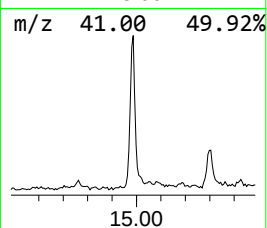
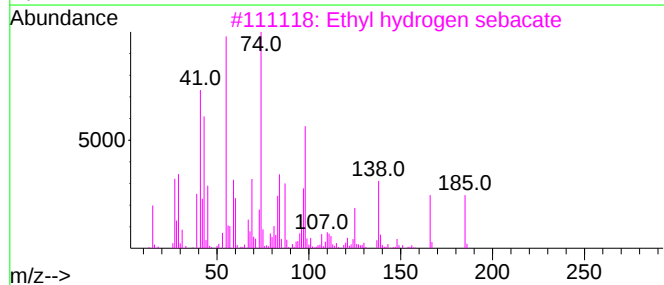
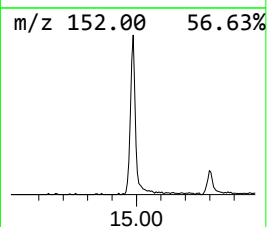
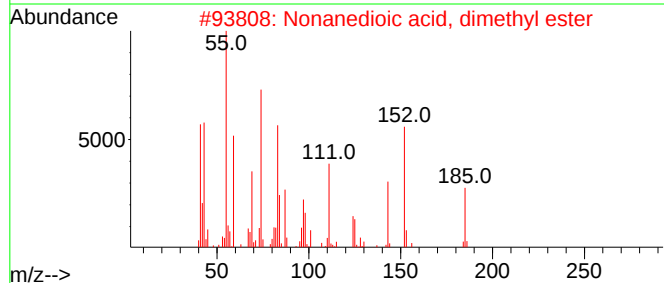
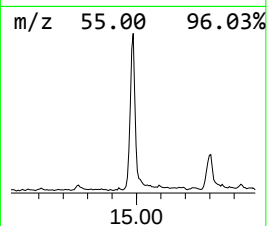
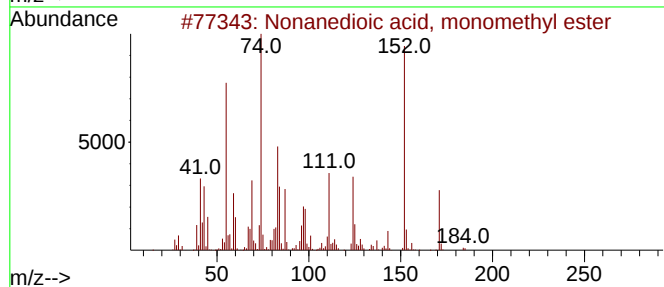
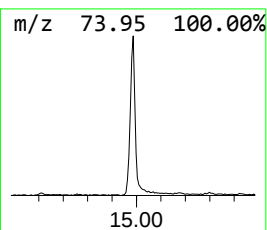
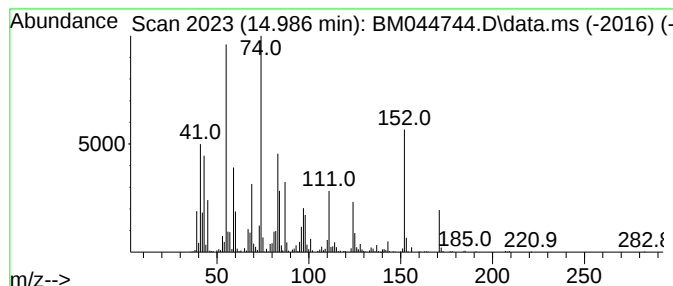
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Peak Number 5 Nonanedioic acid, monomethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	8.03 ng	716082	Acenaphthene-d10	14.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanedioic acid, monomethyl ester	202	C10H18O4	002104-19-0	91
2			Nonanedioic acid, dimethyl ester	216	C11H20O4	001732-10-1	50
3			Ethyl hydrogen sebacate	230	C12H22O4	1010342-39-1	38
4			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	27
5			Nonanoic acid, methyl ester	172	C10H20O2	001731-84-6	22



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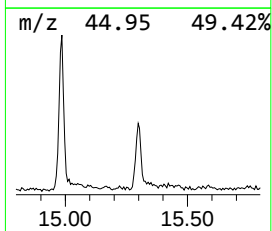
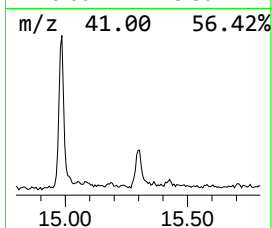
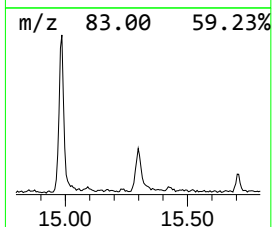
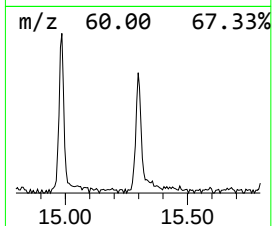
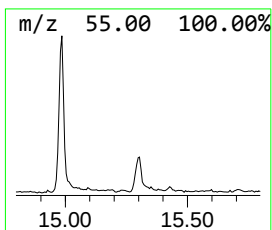
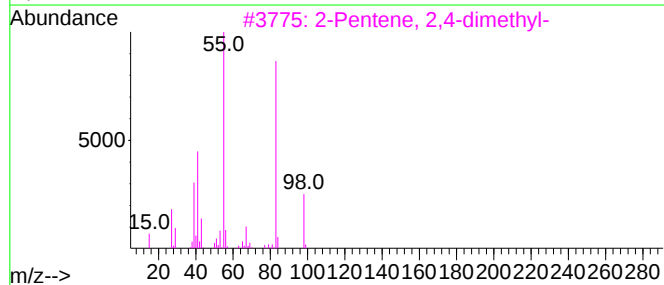
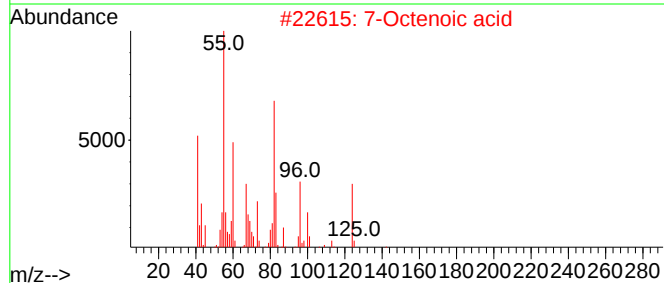
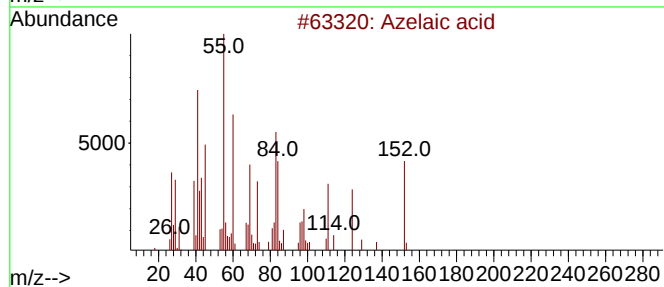
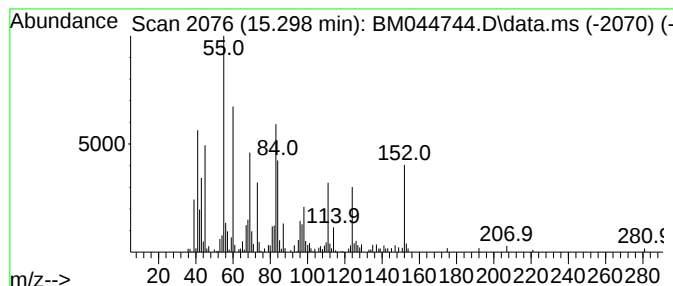
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Azelaic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.298	2.26 ng	201761	Acenaphthene-d10	14.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Azelaic acid	188	C9H16O4	000123-99-9	91
2			7-Octenoic acid	142	C8H14O2	018719-24-9	25
3			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	11
4			5-Hexenoic acid	114	C6H10O2	001577-22-6	11
5			Cyclohexane, methyl-	98	C7H14	000108-87-2	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044744.D
Acq On : 22 Mar 2024 20:52
Operator : MA/JU
Sample : P1788-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PEZOMETER-200

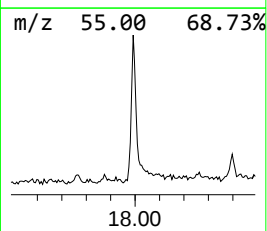
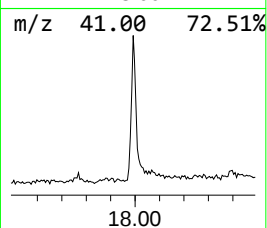
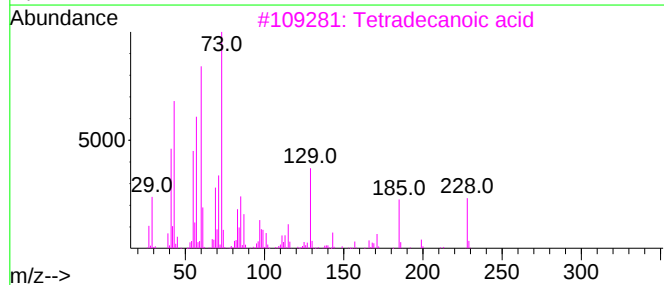
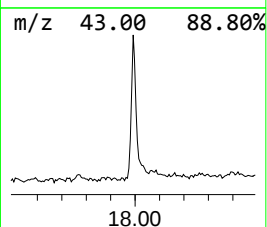
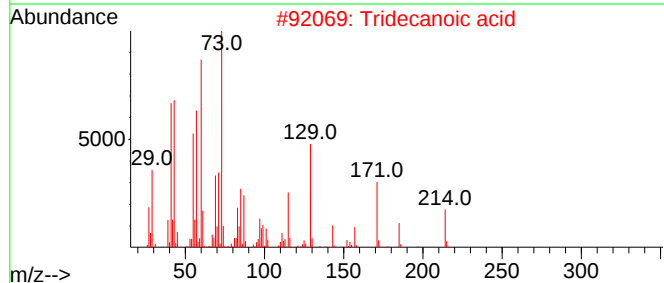
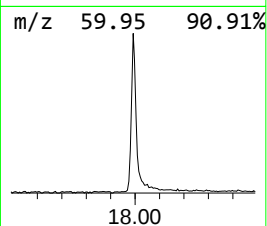
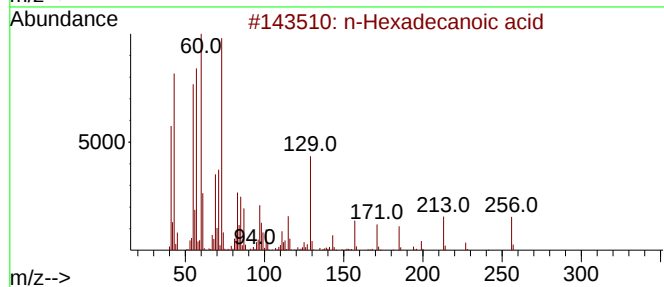
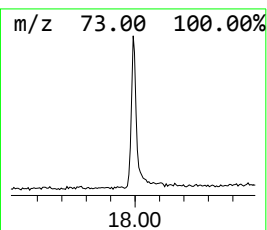
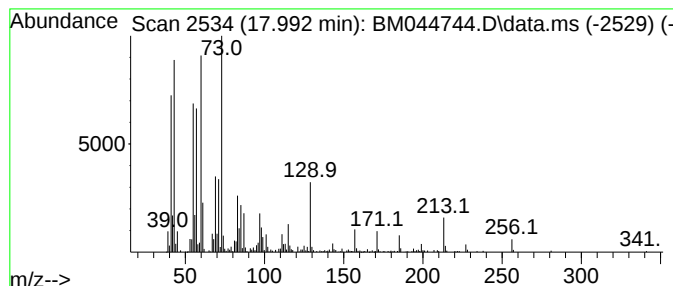
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.992	5.98 ng	549477	Phenanthrene-d10	17.080

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044744.D
Acq On : 22 Mar 2024 20:52
Operator : MA/JU
Sample : P1788-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PEZOMETER-200

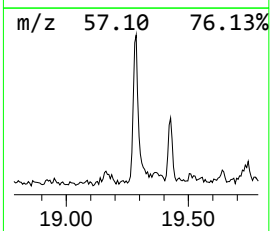
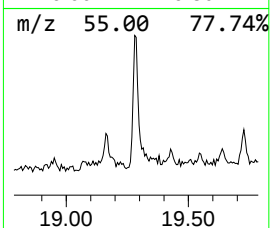
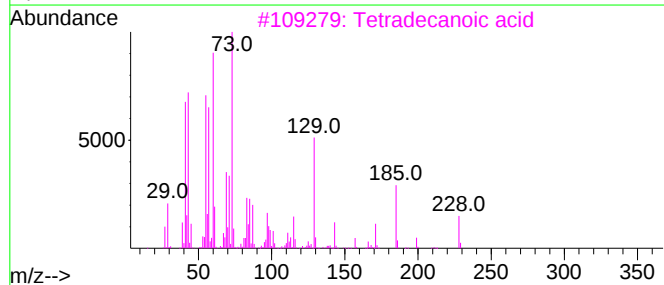
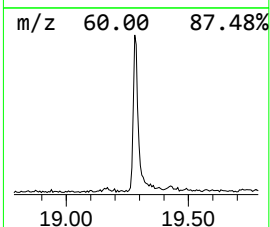
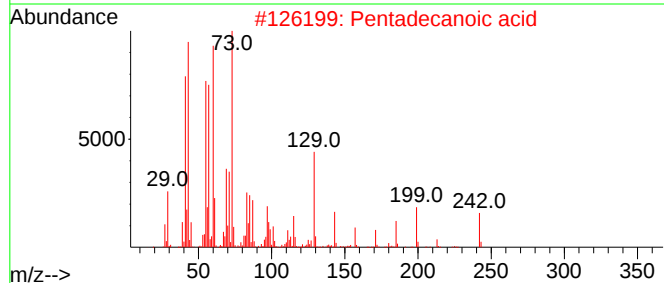
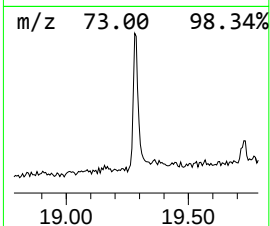
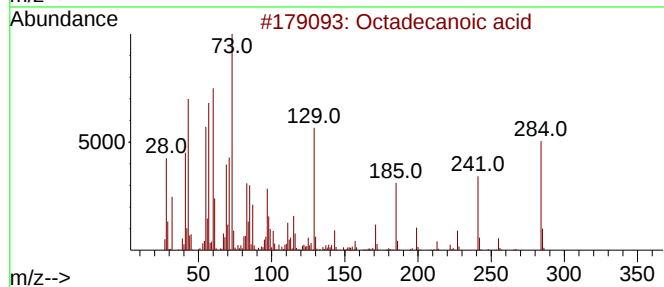
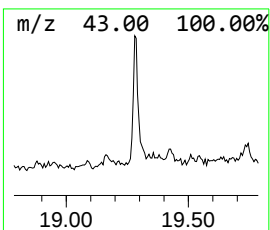
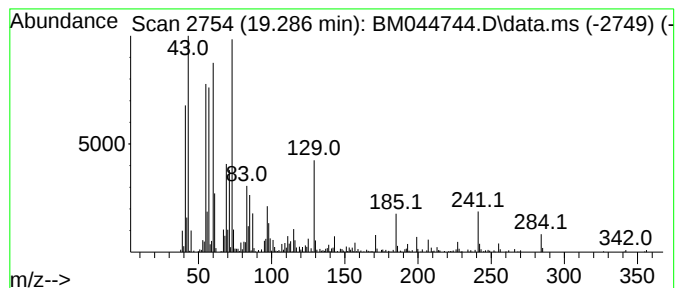
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.286	3.85 ng	369252	Chrysene-d12	21.280

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	90
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
Data File : BM044744.D
Acq On : 22 Mar 2024 20:52
Operator : MA/JU
Sample : P1788-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PEZOMETER-200

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.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-...	4.875	9.1	ng	564695	1	7.687	1237340	20.0
Hexanoic acid, ...	9.040	40.1	ng	2481120	1	7.687	1237340	20.0
Ethanol, 2-(2-b...	10.257	2.6	ng	212153	2	10.463	1659780	20.0
Nonanoic acid, ...	13.551	2.1	ng	188847	3	14.327	1782860	20.0
Nonanedioic aci...	14.986	8.0	ng	716082	3	14.327	1782860	20.0
Azelaic acid	15.298	2.3	ng	201761	3	14.327	1782860	20.0
n-Hexadecanoic ...	17.992	6.0	ng	549477	4	17.080	1838090	20.0
Octadecanoic acid	19.286	3.9	ng	369252	5	21.280	1919800	20.0