

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP021624\
 Data File : BP019745.D
 Acq On : 16 Feb 2024 15:16
 Operator : MA/JU
 Sample : P1440-03
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TW-2

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_P\Methods\8270E-BP013124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.081	164	169	182	rVB	199000	269345	3.72%	1.095%
2	5.022	322	329	339	rBV	46775	73803	1.02%	0.300%
3	5.475	399	406	415	rBV	908793	1345291	18.59%	5.469%
4	7.075	670	678	690	rBV	540810	912898	12.62%	3.711%
5	7.899	810	818	825	rBV	266642	437568	6.05%	1.779%
6	9.075	1010	1018	1025	rBV	913332	1588097	21.95%	6.456%
7	10.698	1287	1294	1308	rBV	310475	561251	7.76%	2.282%
8	13.163	1704	1713	1735	rBV	2493022	3923611	54.22%	15.950%
9	14.534	1939	1946	1957	rBV	466023	759067	10.49%	3.086%
10	16.033	2193	2201	2221	rBV	2157563	3502580	48.40%	14.238%
11	17.298	2409	2416	2426	rBV	652798	1012352	13.99%	4.115%
12	18.192	2563	2568	2576	rBV	127608	219046	3.03%	0.890%
13	19.427	2773	2778	2782	rBV	64134	96939	1.34%	0.394%
14	19.563	2797	2801	2806	rVB	110591	130816	1.81%	0.532%
15	19.863	2846	2852	2865	rBV	5954390	7236579	100.00%	29.418%
16	21.110	3061	3064	3068	rVB2	69163	80117	1.11%	0.326%
17	21.386	3106	3111	3118	rBV	889460	1231755	17.02%	5.007%
18	23.810	3517	3523	3533	rVB	555353	1218418	16.84%	4.953%

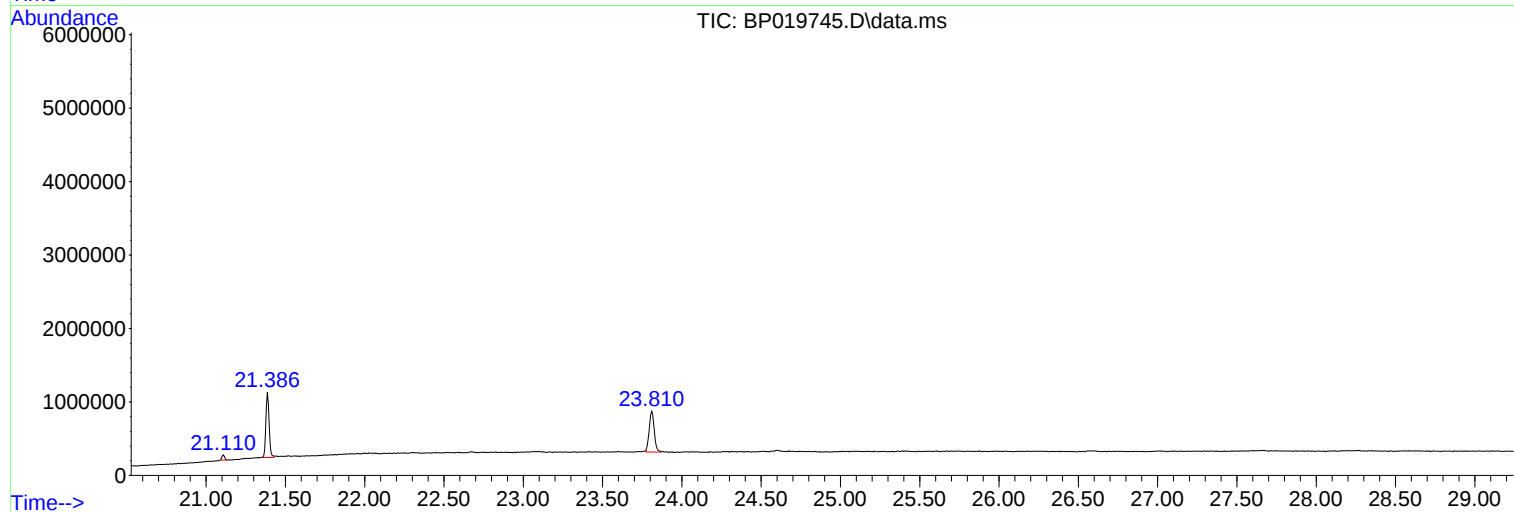
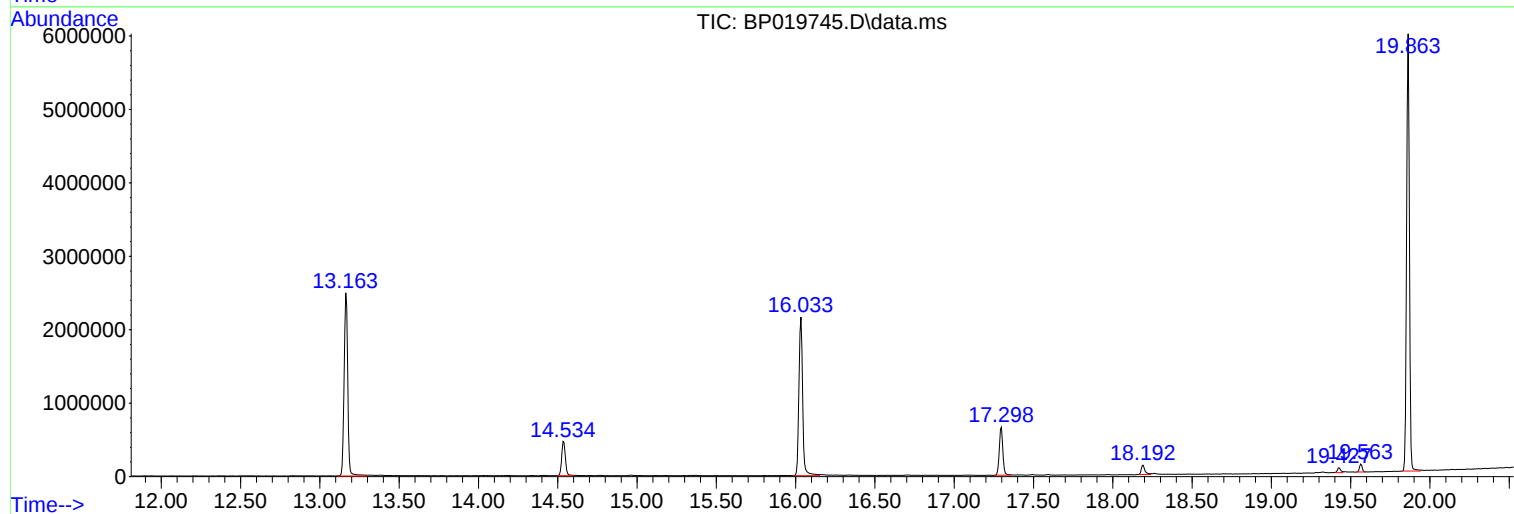
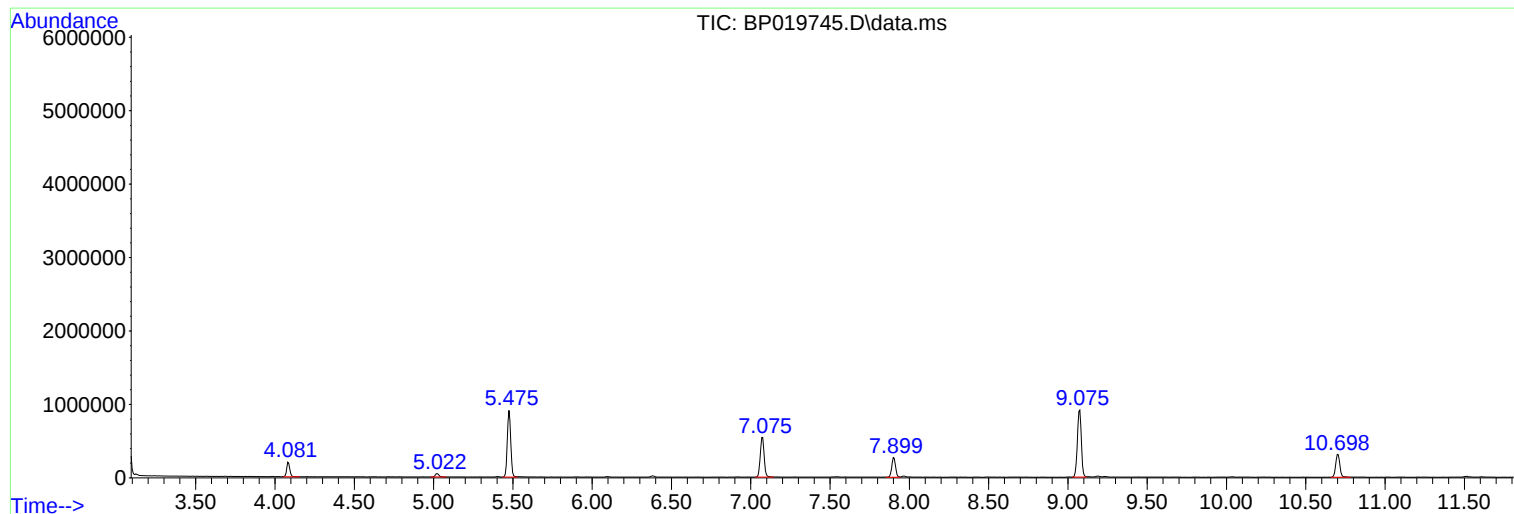
Sum of corrected areas: 24599533

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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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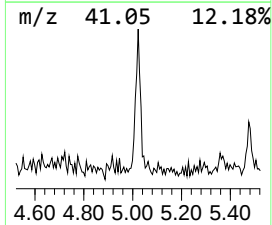
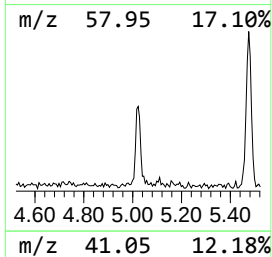
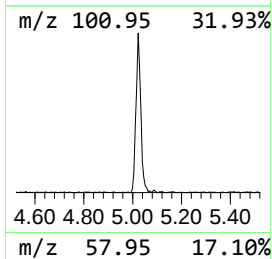
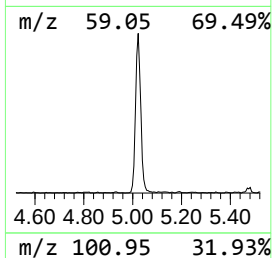
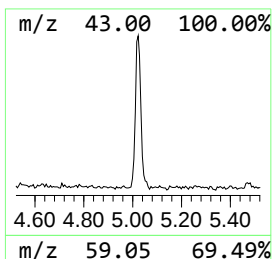
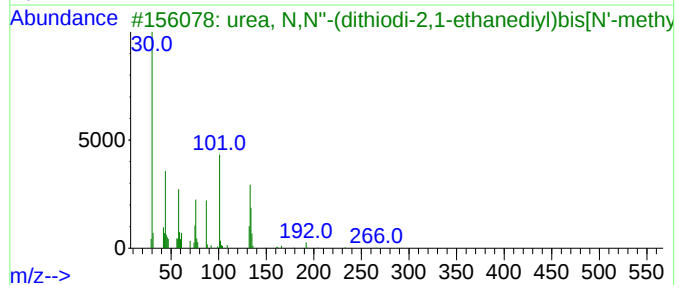
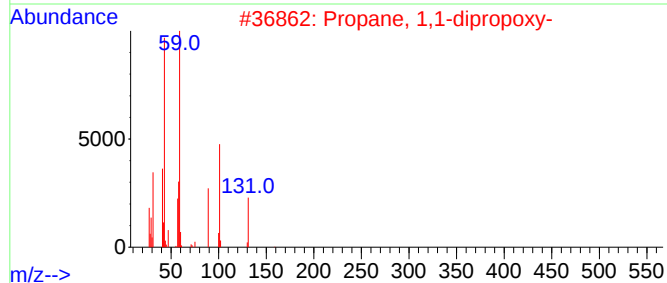
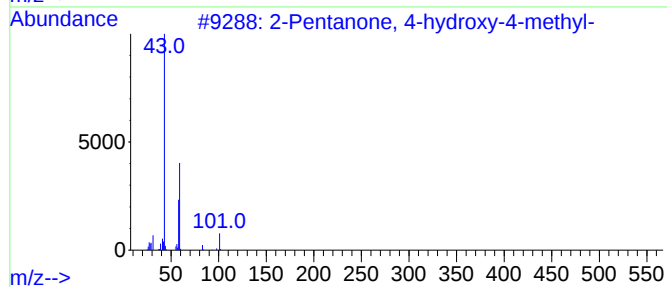
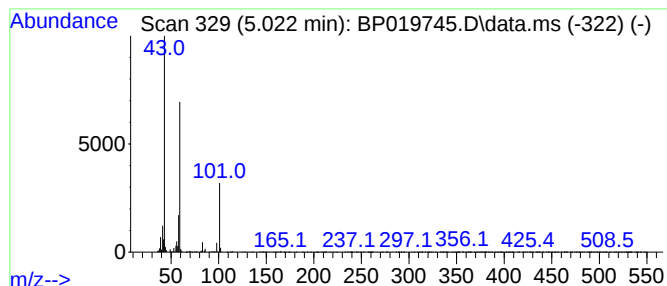
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.37 ng	73803	1,4-Dichlorobenzene-d4	7.899

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3			urea, N,N'-(dithiodi-2,1-ethane...	266	C8H18N4O2S2	1000401-66-6	10
4			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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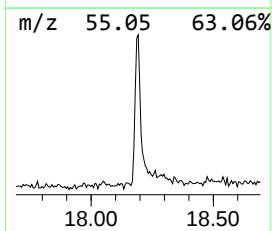
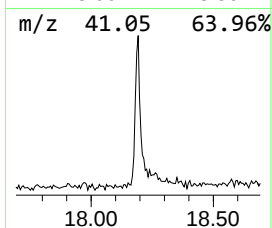
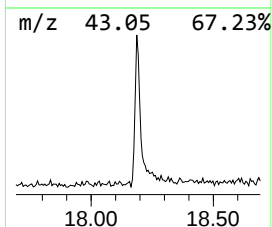
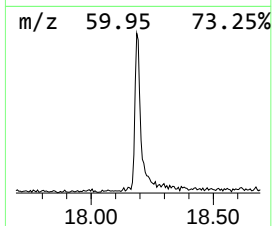
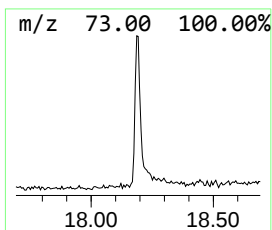
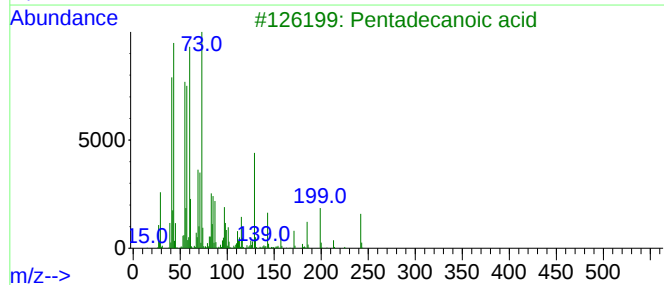
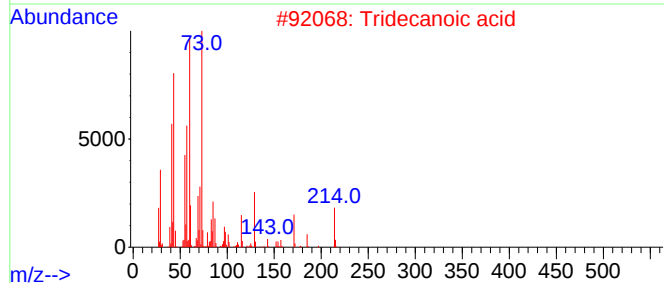
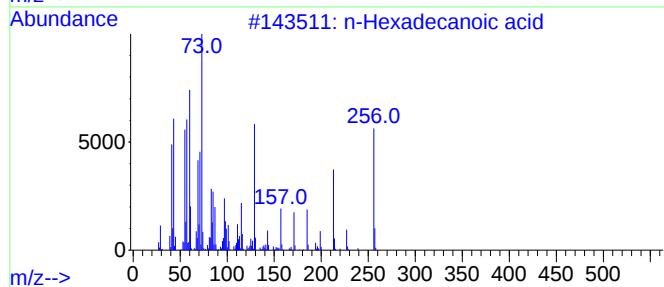
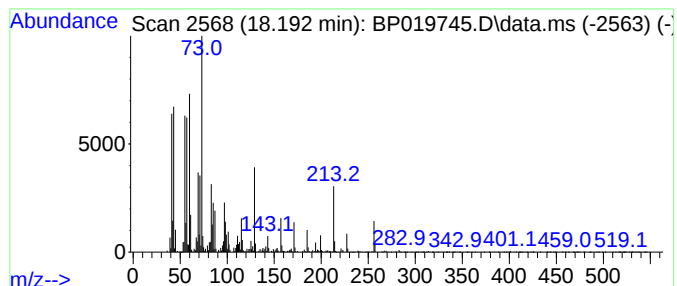
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	4.33 ng	219046	Phenanthrene-d10	17.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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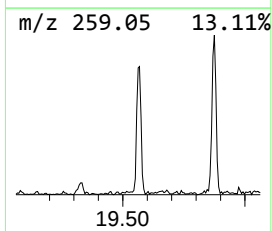
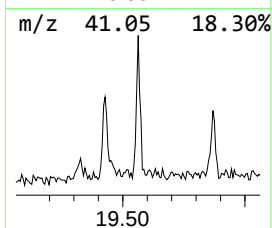
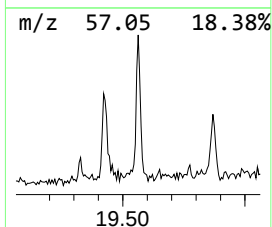
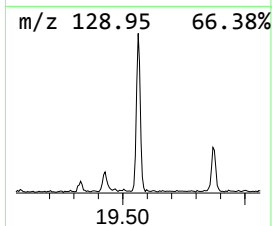
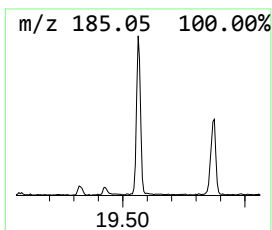
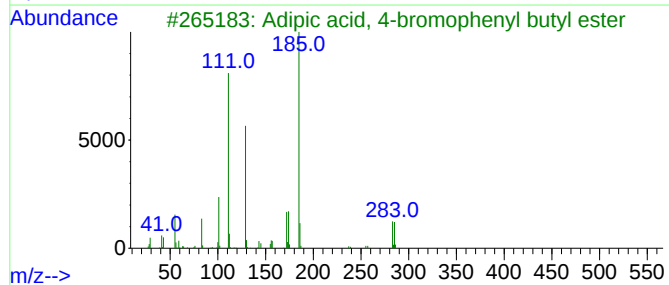
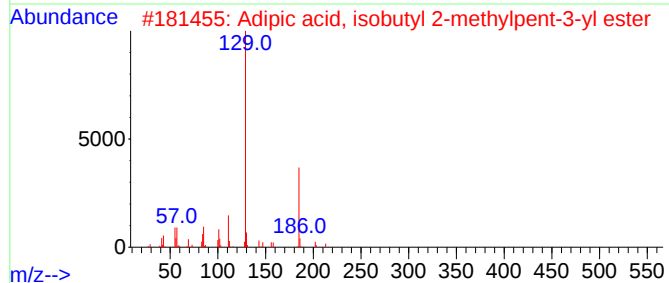
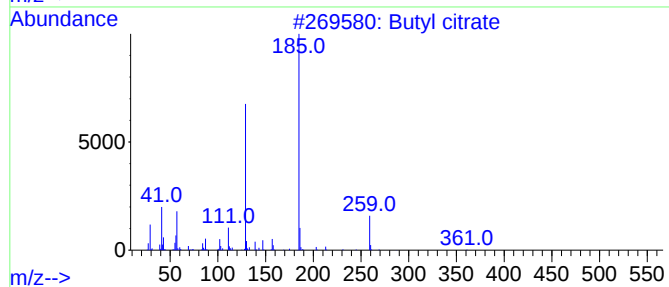
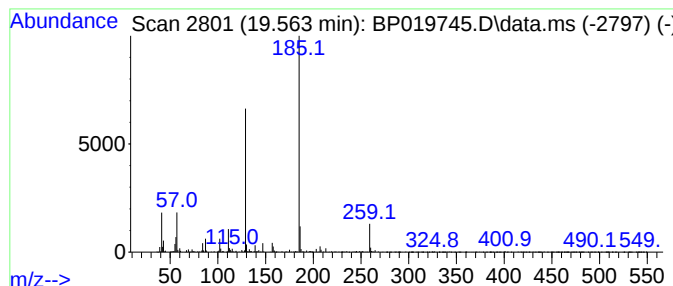
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Peak Number 4 Butyl citrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.563	2.12 ng	130816	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	94
2			Adipic acid, isobutyl 2-methylpe...	286	C16H30O4	1000353-55-7	72
3			Adipic acid, 4-bromophenyl butyl...	356	C16H21BrO4	1000324-37-9	64
4			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	56
5			Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	56



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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-...	5.022	3.4	ng	73803	1	7.899	437568	20.0
n-Hexadecanoic ...	18.192	4.3	ng	219046	4	17.298	1012350	20.0
Butyl citrate	19.563	2.1	ng	130816	5	21.386	1231760	20.0