

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050124\
Data File : BF137791.D
Acq On : 01 May 2024 14:51
Operator : CG\JU
Sample : P2306-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4-20240429

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_F\Methods\8270-BF043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137791.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	17	22	29	rVB2	101112	193696	2.45%	0.450%
2	2.434	53	59	65	rVB	1095776	1465485	18.52%	3.403%
3	5.681	606	611	614	rBV	3464872	3120482	39.43%	7.246%
4	6.663	773	778	781	rBV	2431869	2024102	25.58%	4.700%
5	7.057	841	845	848	rBV	1691559	1343279	16.97%	3.119%
6	7.622	935	941	944	rBV	4099956	4117249	52.03%	9.560%
7	8.339	1059	1063	1066	rBV	2333295	1882919	23.79%	4.372%
8	9.416	1241	1246	1249	rBV	7993178	7913410	100.00%	18.375%
9	10.104	1359	1363	1366	rBV	2834074	2274469	28.74%	5.281%
10	10.898	1493	1498	1501	rBV	5430007	4992068	63.08%	11.591%
11	11.598	1613	1617	1621	rBV	2625845	2180116	27.55%	5.062%
12	12.104	1698	1703	1708	rBV	356636	357699	4.52%	0.831%
13	12.816	1820	1824	1833	rBV	133953	176224	2.23%	0.409%
14	12.892	1834	1837	1845	rVB	140986	150459	1.90%	0.349%
15	13.192	1883	1888	1891	rBV	8004708	7728668	97.67%	17.946%
16	14.251	2064	2068	2071	rBV	1643133	1455699	18.40%	3.380%
17	15.351	2247	2255	2262	rBV4	89857	263035	3.32%	0.611%
18	15.821	2329	2335	2350	rBV	1019876	1427920	18.04%	3.316%

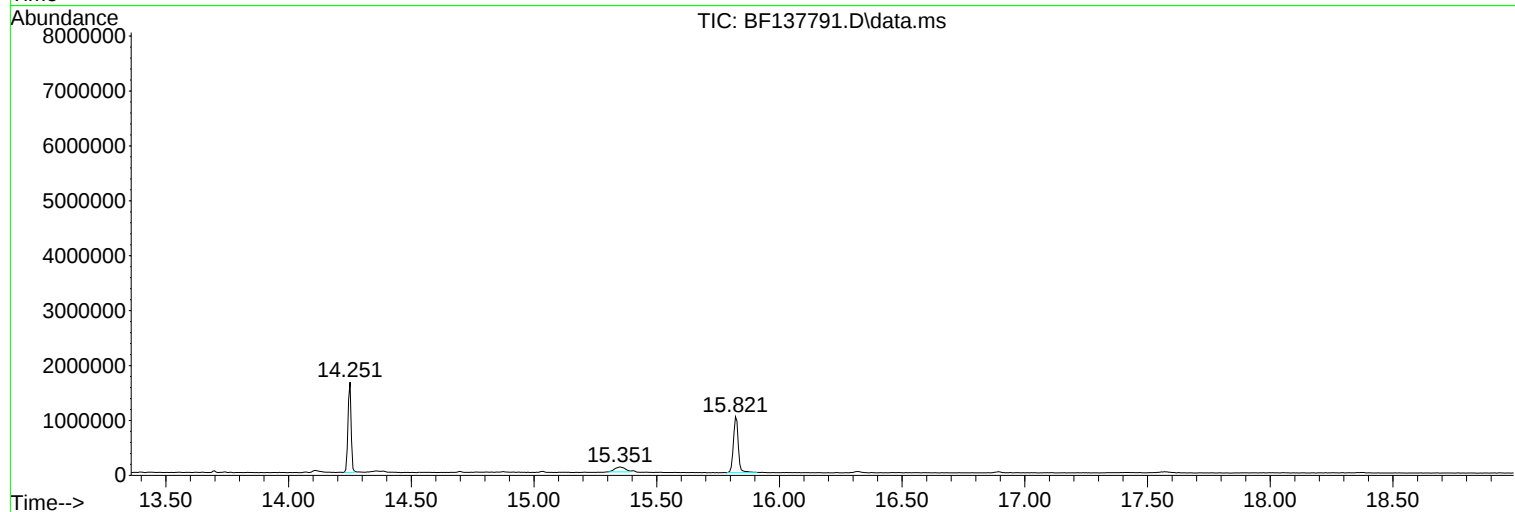
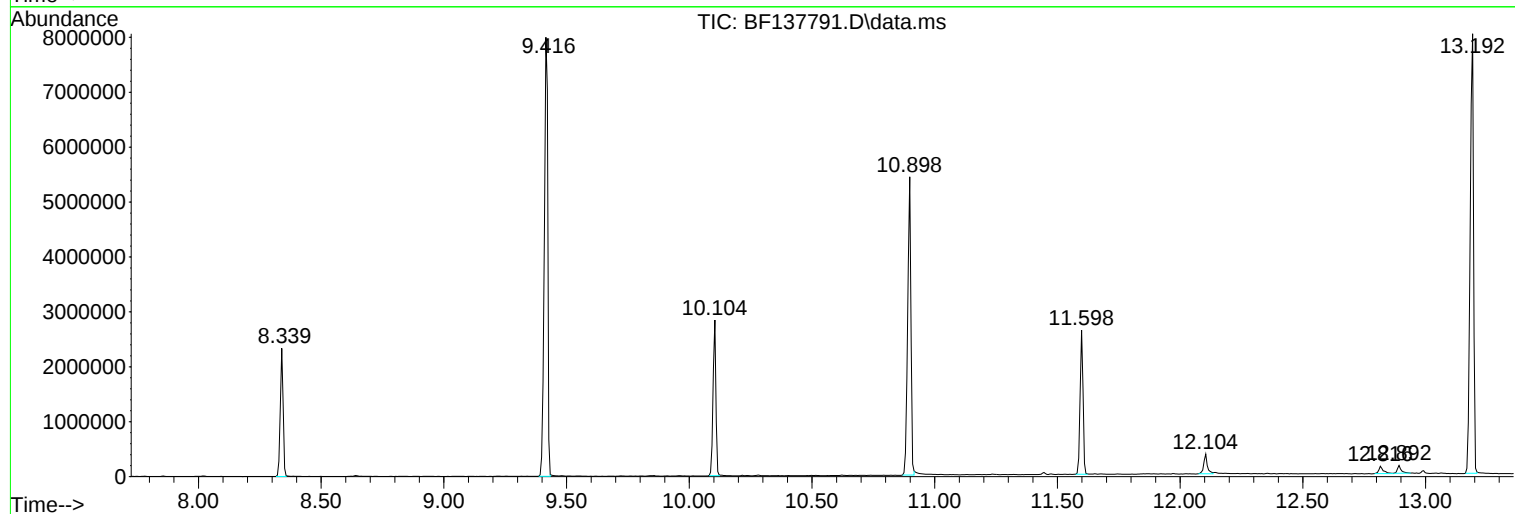
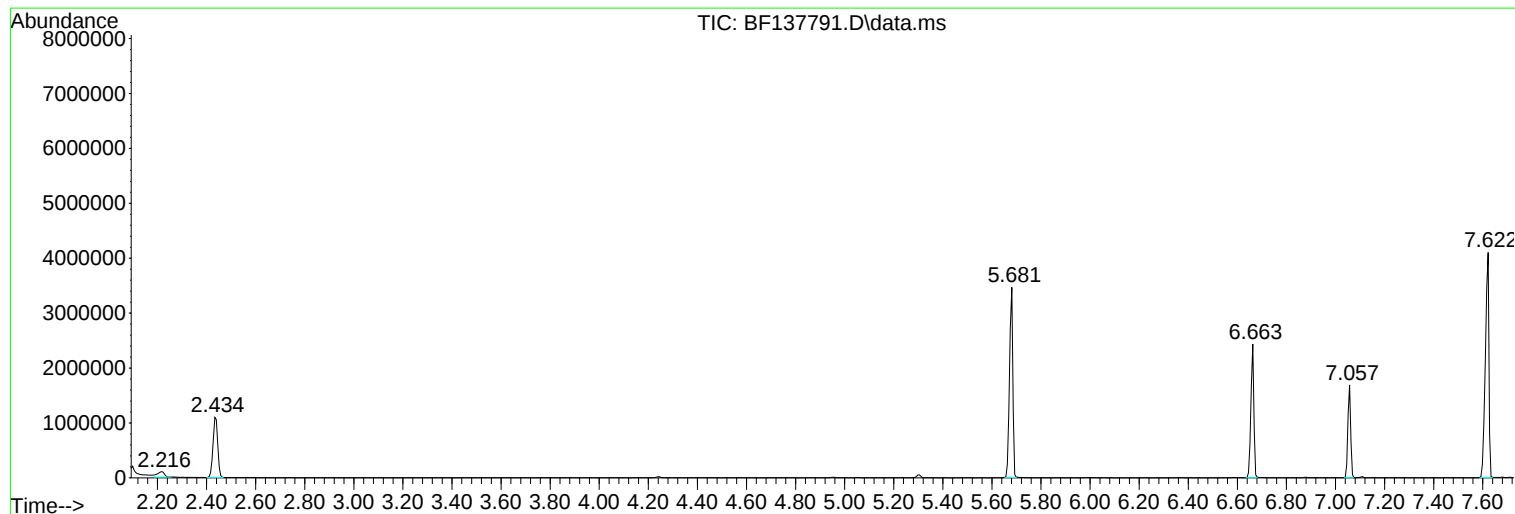
Sum of corrected areas: 43066979

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.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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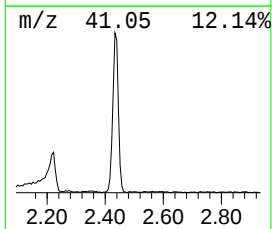
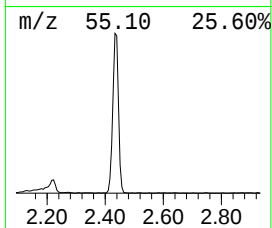
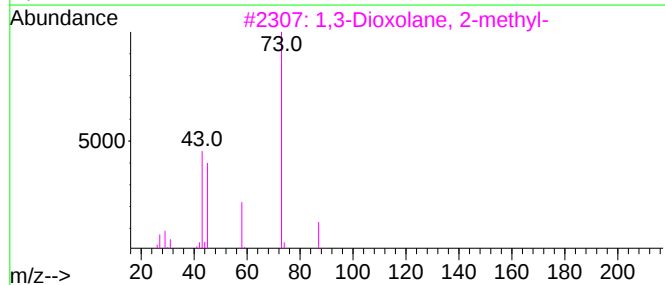
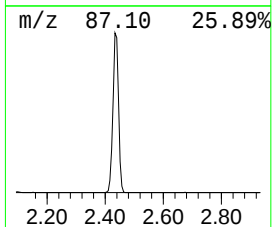
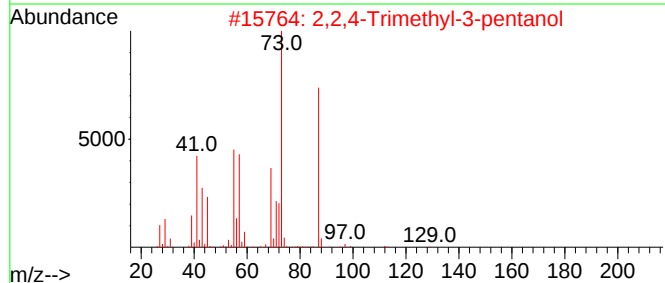
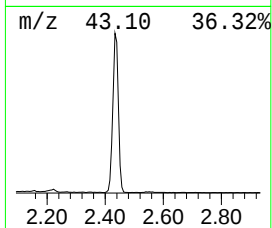
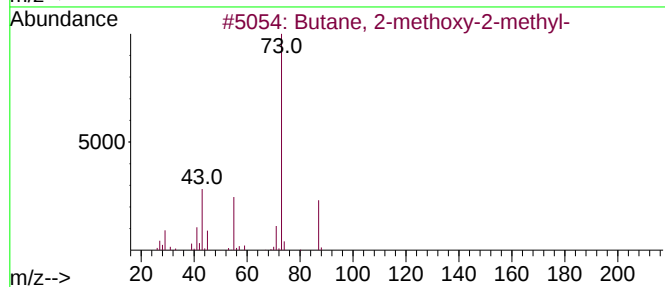
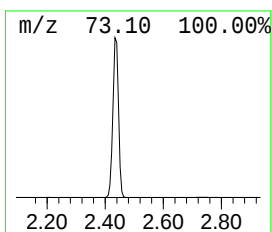
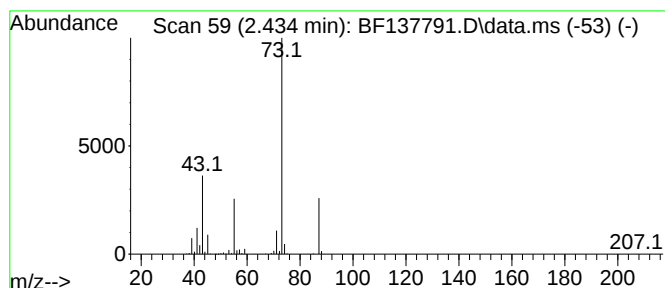
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.434	21.82 ng	1465490	1,4-Dichlorobenzene-d4	7.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22



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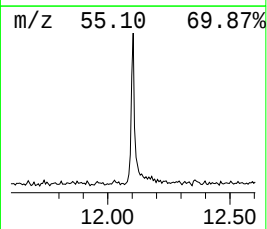
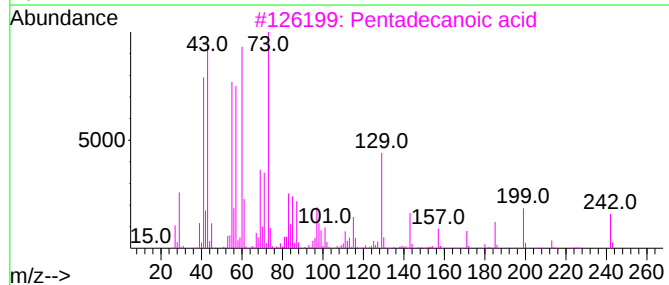
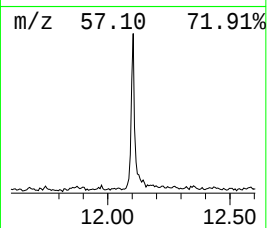
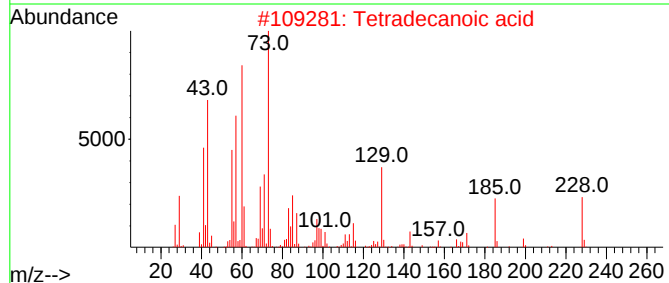
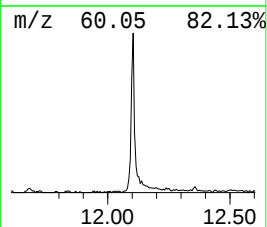
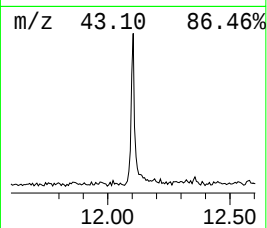
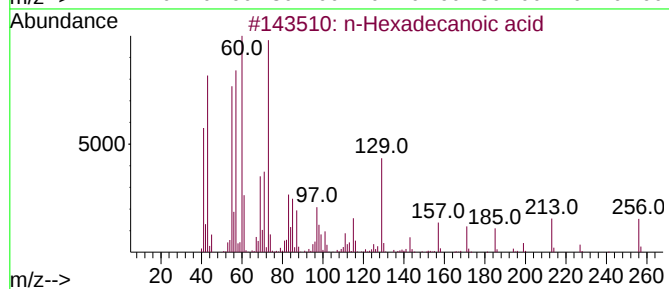
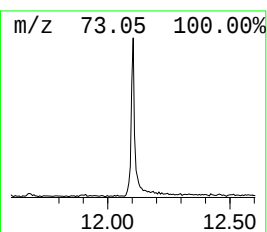
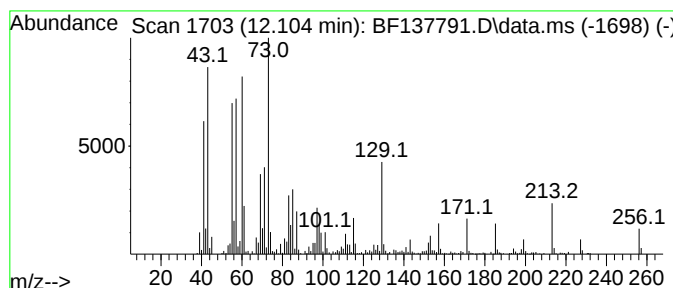
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	3.28 ng	357699	Phenanthrene-d10	11.598

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Undecanoic acid	186	C11H22O2	000112-37-8	87



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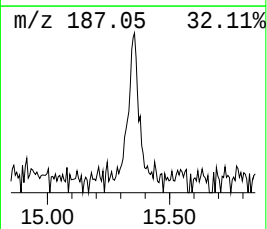
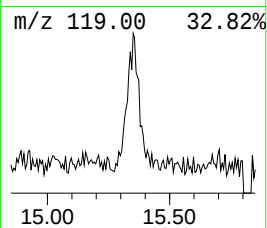
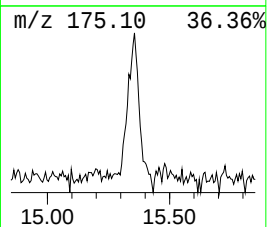
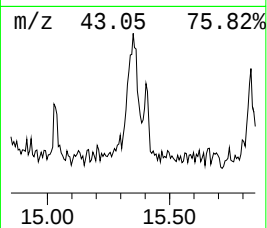
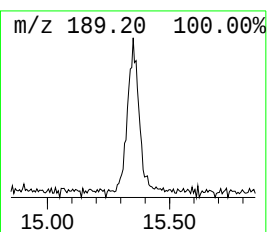
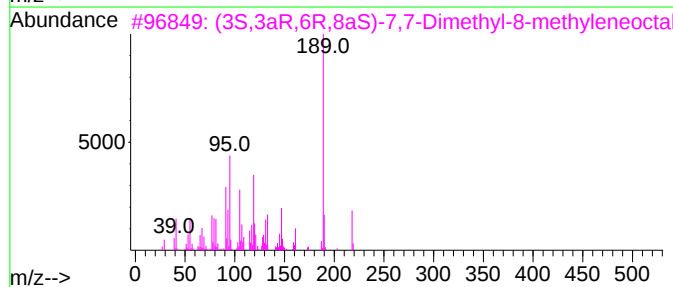
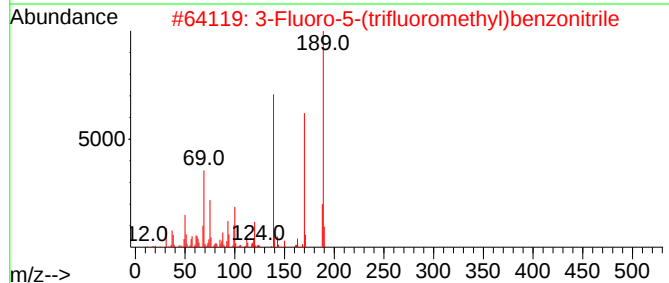
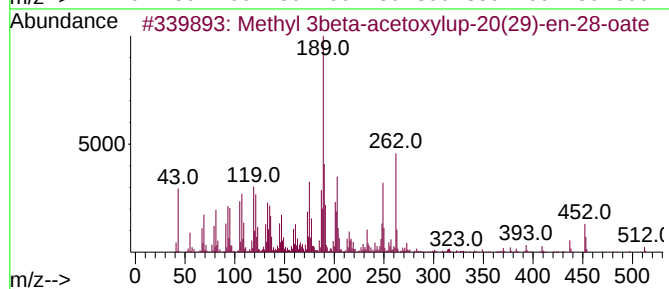
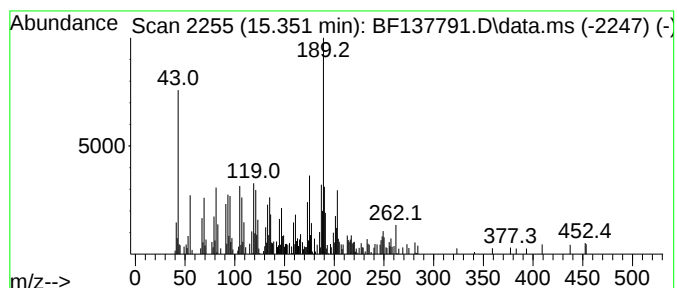
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Peak Number 4 Methyl 3beta-acetoxylup-20(...) Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	3.68 ng	263035	Perylene-d12	15.821

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 3beta-acetoxylup-20(29)-e...	512	C33H52O4	004356-30-3	64
2			3-Fluoro-5-(trifluoromethyl)benz...	189	C8H3F4N	149793-69-1	46
3			(3S,3aR,6R,8aS)-7,7-Dimethyl-8-m...	218	C15H22O	082509-29-3	46
4			2-Fluoro-4-(trifluoromethyl)benz...	189	C8H3F4N	146070-34-0	43
5			Lusitanicoside, hexamethyl ether	526	C27H42O10	1000502-42-3	43



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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
Butane, 2-metho...	2.434	21.8	ng	1465490	1	7.057	1343280	20.0
n-Hexadecanoic ...	12.104	3.3	ng	357699	4	11.598	2180120	20.0
Methyl 3beta-ac...	15.351	3.7	ng	263035	6	15.821	1427920	20.0